mologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in connection with the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mam-5 mal or an insect, but is preferably a microbial cell, e.g. a bacterial or a fungal (including yeast) cell.

Examples of suitable bacteria are Gram positive bacteria such as Bacillus subtilis, Bacillus licheniformis, Bacillus lentus, Bacillus brevis, Bacillus stearothermophilus, Bacillus alkalophilus, Bacillus amyloliquefaciens, Bacillus coagulans, Bacillus circulans, Bacillus lautus, Bacillus megaterium, Bacillus thuringiensis, or Streptomyces lividans or Streptomyces murinus, or gramnegative bacteria such as E.coli. The transformation of the bacteria may, for instance, be effected by protoplast transformation or by using competent cells in a manner known per se.

The yeast organism may favorably be selected from a species of Saccharo-15 myces or Schizosaccharomyces, e.g. Saccharomyces cerevisiae.

The host cell may also be a filamentous fungus e.g. a strain belonging to a species of Aspergillus, most preferably Aspergillus oryzae or Aspergillus niger, or a strain of Fusarium, such as a strain of Fusarium oxysporium, Fusarium graminearum (in the perfect state named Gribberella zeae, previously Sphaeria zeae, synonym with Gibberella roseum and Gibberella roseum f. sp. cerealis), or Fusarium sulphureum (in the prefect state named Gibberella puricaris, synonym with Fusarium trichothecioides, Fusarium bactridioides, Fusarium sambucium, Fusarium roseum, and Fusarium roseum var. graminearum), Fusarium cerealis (synonym with Fusarium crokkwellnse), or Fusarium venenatum.

In a preferred embodiment of the invention the host cell is a protease deficient or protease minus strain.

This may for instance be the protease deficient strain *Aspergillus oryzae* JaL 125 having the alkaline protease gene named "alp" deleted. This strain is described in WO 97/35956 (Novo Nordisk).

Filamentous fungi cells may be transformed by a process involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall in a manner known per se. The use of *Aspergillus* as a host micro-organism is de-

scribed in EP 238 023 (Novo Nordisk A/S), the contents of which are hereby incorporated by reference.

# Method of producing the cutinase variant of the invention

In yet a further aspect, the present invention relates to a method of producing a cutinase variant of the invention, which method comprises cultivating a host cell under conditions conducive to the production of the variant and recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and obtaining expression of the cutinase variant of the invention. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

The cutinase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including separating the cells from the medium by centrifugation or filtration, and precipitating proteinaceous components of the medium by means of a salt such as ammonium sulphate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

# Expression of variant in plants

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The present invention also relates to a transgenic plant, plant part or plant cell which has been transformed with a DNA sequence encoding the variant of the invention so as to express and produce this enzyme in recoverable quantities. The enzyme may be recovered from the plant or plant part. Alternatively, the plant or plant part containing the recombinant enzyme may be used as such.

The transgenic plant can be dicotyledonous or monocotyledonous, for short a dicot or a monocot. Examples of monocot plants are grasses, such as meadow grass (blue grass, Poa), forage grass such as festuca, lolium, temperate grass, such as Agrostis, and cereals, e.g. wheat, oats, rye, barley, rice, sorghum and maize (corn).

Examples of dicot plants are tobacco, legumes, such as lupins, potato, sugar beet, pea, bean and soybean, and cruciferous (family Brassicaceae), such as cauliflower, oil seed rape and the closely related model organism Arabidopsis thaliana.

Examples of plant parts are stem, callus, leaves, root, fruits, seeds, and tubers. In the present context, also specific plant tissues, such as chloroplast, apoplast, mitochondria, vacuole, peroxisomes and cytoplasm are considered to be a plant part. Furthermore, any plant cell, whatever the tissue origin, is considered to be a plant part.

Also included within the scope of the invention are the progeny of such plants, plant parts and plant cells.

The transgenic plant or plant cell expressing the variant of the invention may be constructed in accordance with methods known in the art. In short the plant or plant cell is constructed by incorporating one or more expression constructs encoding the enzyme of the invention into the plant host genome and propagating the resulting modified plant or plant cell into a transgenic plant or plant cell.

Conveniently, the expression construct is a DNA construct which comprises a gene encoding the enzyme of the invention in operable association with appropriate regulatory sequences required for expression of the gene in the plant or plant part of choice. Furthermore, the expression construct may comprise a selectable marker useful for identifying host cells into which the expression construct has been integrated and DNA sequences necessary for introduction of the construct into the plant in question (the latter depends on the DNA introduction method to be used).

The choice of regulatory sequences, such as promoter and terminator sequences and optionally signal or transit sequences is determined, eg on the basis of when, where and how the enzyme is desired to be expressed. For instance, the expression of the gene encoding the enzyme of the invention may be constitutive or inducible, or may be developmental, stage or tissue specific, and the gene product may be targeted to a specific tissue or plant part such as seeds or leaves. Regulatory sequences are eg described by Tague et al, Plant, Phys., 86, 506, 1988.

For constitutive expression the 35S-CaMV promoter may be used (Franck et al., 1980. Cell 21: 285-294). Organ-specific promoters may eg be a promoter from

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storage sink tissues such as seeds, potato tubers, and fruits (Edwards & Coruzzi, 1990. Annu. Rev. Genet. 24: 275-303), or from metabolic sink tissues such as meristems (Ito et al., 1994. Plant Mol. Biol. 24: 863-878), a seed specific promoter such as the glutelin, prolamin, globulin or albumin promoter from rice (Wu et al., Plant and Cell 5 Physiology Vol. 39, No. 8 pp. 885-889 (1998)), a Vicia faba promoter from the legumin B4 and the unknown seed protein gene from Vicia faba described by Conrad U. et al. Journal of Plant Physiology Vol. 152, No. 6 pp. 708-711 (1998), a promotter from a seed oil body protein (Chen et al., Plant and cell physiology vol. 39, No. 9 pp. 935-941 (1998), the storage protein napA promoter from Brassica napus, or any other seed 10 specific promoter known in the art, eg as described in WO 91/14772. Furthermore, the promoter may be a leaf specific promoter such as the rbcs promoter from rice or tomato (Kyozuka et al., Plant Physiology Vol. 102, No. 3 pp. 991-1000 (1993), the chlorella virus adenine methyltransferase gene promoter (Mitra, A. and Higgins, DW, Plant Molecular Biology Vol. 26, No. 1 pp. 85-93 (1994), or the aldP gene promoter 15 from rice (Kagaya et al., Molecular and General Genetics Vol. 248, No. 6 pp. 668-674 (1995), or a wound inducible promoter such as the potato pin2 promoter (Xu et al, Plant Molecular Biology Vol. 22, No. 4 pp. 573-588 (1993).

A promoter enhancer element may be used to achieve higher expression of the enzyme in the plant. For instance, the promoter enhancer element may be an intron which is placed between the promoter and the nucleotide sequence encoding the enzyme. For instance, Xu et al. *op cit* disclose the use of the first intron of the rice actin 1 gene to enhance expression.

The selectable marker gene and any other parts of the expression construct may be chosen from those available in the art.

The DNA construct is incorporated into the plant genome according to conventional techniques known in the art, including *Agrobacterium*-mediated transformation, virus-mediated transformation, micro injection, particle bombardment, biolistic transformation, and electroporation (Gasser et al, Science, 244, 1293; Potrykus, Bio/Techn. 8, 535, 1990; Shimamoto et al, Nature, 338, 274, 1989).

Presently, Agrobacterium tumefaciens mediated gene transfer is the method of choice for generating transgenic dicots (for review Hooykas & Schilperoort, 1992. Plant Mol. Biol. 19: 15-38), however it can also be used for transforming monocots,

although other transformation methods are generally preferred for these plants. Presently, the method of choice for generating transgenic monocots is particle bombardment (microscopic gold or tungsten particles coated with the transforming DNA) of embryonic calli or developing embryos (Christou, 1992. Plant J. 2: 275-281; Shimamoto, 1994. Curr. Opin. Biotechnol. 5: 158-162; Vasil et al., 1992. Bio/Technology 10: 667-674). An alternative method for transformation of monocots is based on protoplast transformation as described by Omirulleh S, et al., Plant Molecular biology Vol. 21, No. 3 pp. 415-428 (1993).

Following transformation, the transformants having incorporated the expres-10 sion construct are selected and regenerated into whole plants according to methods well-known in the art.

#### **MATERIALS AND METHODS**

#### **Plasmids**

#### pJSO026

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This is a *S. cerevisiae* expression plasmid described in WO 97/07205 and in J.S.Okkels, (1996) "A URA3-promoter deletion in a pYES vector increases the expression level of a fungal lipase in Saccharomyces cerevisiae. Recombinant DNA Biotechnology III: The Integration of Biological and Engineering Sciences, vol. 782 of the Annals of the New York Academy of Sciences).

#### 20 pFuku83

This is a yeast and E. coli shuttle vector for expression of the H. insolens cutinase under the control of a TPI promoter, constructed from pJSO026.

#### **Substrate**

#### **BETEB**

Terephthalic acid bis(2-hydroxyethyl)ester dibenzoate is herein abbreviated as BETEB (benzoyl-ethylene-terephthalic-ethelene-benzoate). It was prepared from terephthalic acid bis (2-hydroxyethyl) ester and benzoic acid.

# Lipase activity (LU)

A substrate for lipase is prepared by emulsifying tributyrin (glycerin tributyrate) using gum Arabic as emulsifier. The hydrolysis of tributyrin at 30 °C at pH 7 is followed in a pH-stat titration experiment. One unit of lipase activity (1 LU) equals the amount of enzyme capable of releasing 1 µmol butyric acid/min at the standard conditions.

# Differential scanning calorimetry (DSC)

Sample and reference solutions are carefully degassed immediately prior to loading of samples into the calorimeter (reference: buffer without enzyme). Sample and reference solutions (approx. 0.5 ml) are thermally pre-equillibrated for 20 minutes at 5°C. The DSC scan is performed from 5 C to 95 C at a scan rate of approx. 90 K/hr. Denaturation temperatures are determined at an accuracy of approx. +/- 1 C. A VP-DSC from MicroCal Inc. is suitable for the experiments.

#### Methods

# 15 PCR conditions

step 1: 94° C, 120 sec.

step 2: 94° C, 60 sec

step 3: 50° C, 60 sec

step 4: 72° C, 150 sec.

20 Go to step 2, 35 cycles

step 5: 72° C, 480 sec.

Step 6: 4° C, for ever

#### **EXAMPLES**

#### Example 1

# Preparation of cutinase variants

A DNA sequence encoding *H. insolens* cutinase was obtained as described in 5 US 5,827,719 (Novo Nordisk) and was found to have the DNA sequence shown in SEQ ID NO: 1 therein.

Variants were prepared by localized random mutagenesis and selection of positive clones by incubation at 60°C for 1 day on BETEB plates. The BETEB plates contained 200 ml/l of 500 mM glycine buffer (pH 8.5), 1.25 g/l of BETEB (dissolved in hot ethanol) and 20 g/l of agar.

Three positive variants (denoted JC013, JC014, JC025) were isolated, and their amino acid sequence was determined. They were found to have the following modifications, compared to the parent *H. insolens* cutinase:

JC013: A14P + E47K

JC014: E47K

JC025: E179Q

# Example 2

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#### Site directed mutation

JC026 (E6Q, E47K, R51P) was prepared as follows:

A pair of PCR primers were designed so as to introduce amino acid substitutions, making use of the existed restriction enzyme sites nearby, as follows (an asterisk indicates an introduced mutation):

Upper primer: E6Q F

cgg cag ctg gga gcc atc c\*ag aac

25 Pvu ||

Lower primer: E47K,R51P

cgc cct gga tcc aga tgt tcg\* gga tgt ggg act t\*aa ggc

BamH I

PCR was run using these primers and pFukuNL83 as a template under the PCR condition described above.

The obtained PCR fragment was purified by Clontech Spincolumn and digested with *Pvu* II and *Bam*H I.

The resultant fragment was gel-purified and ligated to pFukuNL83 which had been digested with the same restriction enzyme sites.

# Example 3

# Thermostability of cutinase variants

Thermostability of cutinase variants was investigated by means of DSC (Differential Scanning Calorimetry) at pH 4.5 (50 mM acetate buffer) and pH 8.5 (50mM glycyl-glycine buffer). The thermal denaturation temperature, Td, was taken as the top of denaturation peak (major endothermic peak) in thermograms (Cp vs. T) obtained after heating of enzyme solutions at a constant programmed heating rate. The parent cutinase (NL83) was included for comparison. Results:

|               | pH 4.5 | pH 8.5 |
|---------------|--------|--------|
| JC013         | -      | 70     |
| JC014         | -      | 70     |
| JC015         | 65     | 70     |
| JC026         | 64     | 71     |
| JC029         | 66     | 73     |
| JC038         | 64     | 71     |
| JC039         | 66     | 73     |
| NL83 (parent) | 61     | 63     |

The results show improved thermostability in all cases. The improvement is seen to be 3-5° at pH 4.5, and 7-10° at pH 8.5.

#### Example 4

# Hydrolysis of BETEB

The thermostability of *H, insolens* cutinase variants JC014 (E47K) and JC025 (E179Q) was measured by hydrolysis of BETEB at elevated temperature. The parent

cutinase (denoted NL83) was tested for comparison. For each cutinase, the following mixture was incubated for 17 hours at various temperatures in the range 55-70°C::

- 0.1 ml 0.5 M glycyl-glycine buffer (pH 8.5)
- 0.1 ml 0.5 % BETEB dissolved in ethanol
- 0.1 ml enzyme solution (approx. 25 LU/ml)
- 0.7 ml Milli Q water

The degree of hydrolysis was measured after the incubation. The results are shown in the table below.

|        | JC014    | JC025    | NL83 (parent) |
|--------|----------|----------|---------------|
|        | 27 LU/ml | 25 LU/ml | 24 LU/mi      |
| 55°C   | 98 %     | 99 %     | 72 %          |
| . 60°C | 91 %     | 83 %     | 33 %          |
| 65°C   | 66 %     | 13 %     | 7 %           |
| 70°C   | 6 %      | 6 %      | 7 %           |

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These results clearly show that the variants have improved thermostability compared to the parent cutinase.

# Example 5 Hydrolysis of BETEB

The thermostability of cutinase variants JC013, JC038 and JC039 was measured by hydrolysis of BETEB at 60°C for 2 hours. The parent cutinase (denoted NL83) was tested for comparison. The hydrolysis was carried out at the same conditions as in Example 2, except that the temperature was fixed at 60°C and the cutinase dosage was varied. The results below are shown in the table below.

| LU/ml | JC038 | JC039 | JC013 | NL83 (parent) |
|-------|-------|-------|-------|---------------|
| 0     | 0 %   | 0 %   | 0 %   | 0 %           |
| 10    | 97 %  | 99.%  | 9 %   | 6 %           |
| 20    | 98 %  | 99 %  | 74 %  |               |
| 50    | 98 %  | 94 %  | 93 %  | 15 %          |
| 100   | 88 %  | 69 %  | 92 %  | 34 %          |

| 300  | 41 % |
|------|------|
| 600  | 63 % |
| 1200 | 82 % |

The results show a much faster hydrolysis at 60°C with the variants than with the parent cutinase.

# Example 6

# 5 Hydrolysis of c3ET

The thermostability of variants was measured by hydrolysis of c3ET at elevated temperature. Wild type (NL83) was tested for comparison. For each cutinase, the following mixture was incubated for 2 hours at various temperatures.

0.115mg c3ET (0.1ml of 2mM c3ET dissolved in HFIP was taken in reaction vessel. Solvent was removed under vacuum, then dried up at 70°C over night)

0.1ml 0.5M glycyl-glycine buffer (pH8.5)

0.1ml enzyme solution (approx. 600LU/ml)

0.8ml Milli Q water

After the incubation, 2ml of 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) was added to each reaction mixture, then hydrolysis ratio was measured by HPLC. The results shown in Fig 3 clearly indicate the variants especially JC039 have improved thermostability compared to the parent cutinase.

# Example 7

#### Hydrolysis of c3ET on yarn

Similar experiment to the previous example was done using polyester yarn containing c3ET as by product. The following substrate mixture was preincubated at 60 or 65°C:

0.1g polyester yarn

0.2ml 0.5M glycyl-glycine buffer (pH8.5)

25 1.7ml Milli Q water

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After preincubation, 0.1ml enzyme solution (approx. 1000 LU/ml) was added to each reaction vessel and incubated for 17 hours. Then 2ml HFIP was added and

left for 30 minutes to extract and hydrolyze c3ET sitting on the surface of the polyester yarn; then the hydrolysis ratio was measured. The results are shown in Fig. 4.

It is seen that the variants are more effective than the parent cutinase for hy-5 drolyzing c3ET on polyester yarn, particularly JC039. It is also seen that JC039 gives higher hydrolysis ratio at 65°C than 60°C.

# Example 8

# Treatment of yarn by variant JC039

Time courses of c3ET hydrolysis on polyester yarn at different temperature or dosage were examined. Time course at different temperatures is shown in Fig 5. It is seen that optimal temperature of JC039 is 65°C. At 70°C there is still about half of the activity left. Time course with increased enzyme dosage is shown in Fig 6. The curves at dosage 275 and 550 LU/ml are seen to be the same, indicating that the hydrolysis ratio reached to plateau between dosage of 100 to 275 LU/ml. Presumably 200LU/ml is enough.

#### **CLAIMS**

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- 1. A variant of a parent fungal cutinase, which variant:
  - comprises substitution of one or more amino acid residues at a position which is located:
    - within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
    - ii) within 20 positions from the N-terminal amino acid, and
  - b) is more thermostable than the parent cutinase.
- 2. The variant of the preceding claim which comprises substitution of one or more amino acid residues at a position which is located:
  - within 12 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
  - ii) within 15 positions from the N-terminal amino acid.
- 3. A variant of a parent fungal cutinase comprising substitution of one or more amino acid residues which is located:
  - a) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
  - b) within 20 positions from the N-terminal amino acid,

with the proviso that it is not a variant of the cutinase of *Fusarium solani pisi* having one of the substitutions R17, T18, T19V, D21N, I24E, Y38F, R40, G41A, S42, T43, E44, T45, G46, N47R, G49, T50, L51, P53, S54, A56C, S57, N58R, S61, A62E, K65A, D66S, G67D, W69Y, I70C, G74, G75, R78, Y119, G192, P193, D194R, A195, R196, G197V, or A199C (*Fusarium solani pisi* cutinase numbering).

- A variant of a parent fungal cutinase comprising substitution of one or more
   amino acid residues which:
  - a) has a solvent accessible surface, and
  - b) is located:

- i) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
- ii) within 20 positions from the N-terminal amino acid,

with the proviso that it is not a variant of the cutinase of *Fusarium solani pisi* 5 having one of the substitutions T18, Y38F, R40, G41A, S42, T43, E44, T45, N47R, G49, T50, L51, P53, S54, A56C, A62E or G192 (*Fusarium solani pisi* cutinase numbering).

- 5. A variant of a parent fungal cutinase comprising substitution of one or more amino acid residues which is located:
- a) less than 12 Å from the location of the N-terminal amino group (as calculated from amino acid residues in a crystal structure), and/or
  - b) within 15 positions from the N-terminal amino acid,

with the proviso that the variant is not the cutinase of *Fusarium solani pisi* having one of the substitutions R17, T18, T19V, D21N, Y38F, R40, T45, G46, N47R,

- 15 G49, T50, L51, P53, S54, A56C, S57, N58R, K65A or I70C (Fusarium solani pisi cutinase numbering).
  - 6. The variant of any preceding claim wherein the parent cutinase is native to a filamentous fungus, preferably a strain of *Humicola* or *Fusarium*, preferably *H. insolens* or *F. solani pisi*, most preferably *H. insolens* strain DSM 1800.
- The variant of any preceding claim wherein the parent cutinase has an amino acid sequence which can be aligned with the cutinase of *H. insolens* strain DSM 1800.
- The variant of any preceding claim wherein the parent cutinase has an amino acid sequence which is at least 50 % homologous to the cutinase of *H. insolens* strain
   DSM 1800, preferably at least 70 % homologous, more preferably at least 80 % homologous.
  - 9. A variant of a parent fungal cutinase from *Humicola insolens* which comprises substitution of one or more amino acid residues located:

- a) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
- b) within 20 positions from the N-terminal amino acid.
- 10. The variant of the preceding claim which comprises substitution of one or more amino acid residues located:
  - a) less than 12 Å from the location of the N-terminal amino group (as calculated from amino acid residues in a crystal structure), and/or
  - b) within 15 positions from the N-terminal amino acid
- 11. The variant of any preceding claim which comprises substitution of one or more amino acids having a solvent accessible surface.
  - 12. The variant of any preceding claim wherein one or more substitutions is substitution of a negatively charged amino acid with a neutral or positively charged amino acid or substitution of a neutral amino acid with a positively charged amino acid.
  - 13. The variant of any preceding claim wherein one or more substitutions is sub-15 stitution with a Pro residue.
  - 14. The variant of any preceding claim wherein one or more substitutions is at a position corresponding to position E6, E10, A14, E47, R51 and/or E179 in the cutinase of *Humicola insolens* strain DSM 1800, preferably a substitution corresponding to E6Q, E10Q, A14P, E47K, R51P and/or E179Q (*H. insolens* cutinase numbering).
    - 15. The variant of any preceding claim which has one, two, three, four, five or six of said substitutions.
    - 16. The variant of any preceding claim which has substitutions corresponding to one of the following in the cutinase of *Humicola insolens* strain DSM 1800:
  - 25 a) R51P
    - b) E6Q, L138I

- c) A14P, E47K
- d) E47K
- e) E179Q
- f) E6Q, E47K, R51P
- 5 g) A14P, E47K, E179Q
  - h) E47K, E179Q
  - i) E47K, D63N
  - j) E6Q, A14P, E47K, R51P, E179Q
  - k) E6Q, E10Q, A14P, E47K, R51P, E179Q, or
- 10 I) Q1P, L2V, S11C, N15T, F24Y, L46I, E47K
  - 17. The variant of any preceding claim which has hydrolytic activity towards terephthalic acid esters, particularly towards cyclic tri(ethylene terephthalate) and/or Terephthalic acid bis(2-hydroxyethyl)ester dibenzoate (BETEB).
- 18. The variant of any preceding claim which has a denaturation temperature which is at least 5° higher than the parent cutinase, preferably measured at pH 8.5
  - 19. A DNA sequence encoding the variant of any preceding claim.
  - 20. A vector comprising the DNA sequence of the preceding claim.
  - 21. A transformed host cell harboring the DNA sequence of claim 19 or the vector of claim 20.
- 20 22. A method of producing the variant of any of claims 1-18 comprising
  - a) cultivating the cell of claim 21 so as to express and preferably secrete the variant, and
  - b) recovering the variant.
  - 23. A method of constructing a cutinase variant, which method comprises:
- a) selecting a parent fungal cutinase,

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e)

f)

g)

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b) identifying one or more amino acid residues in the parent cutinase at positions which are: i) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or ii) within 20 positions from the N-terminal amino acid, and c) making alterations each of which is an insertion, a deletion or a substitution of the amino acid residue, d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b), e) preparing the variant resulting from steps b-d, f) testing the thermostability of the variant, g) optionally repeating steps b-f, and h) selecting a variant having higher thermostability than the parent cutinase. A method of producing a cutinase variant, which method comprises: a) selecting a parent fungal cutinase, b) identifying one or more amino acid residues in the parent cutinase at positions which are: i) within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or ii) within 20 positions from the N-terminal amino acid, and c) making alterations each of which is an insertion, a deletion or a substitution of the amino acid residue, d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b).

preparing the variant resulting from steps b-d,

testing the thermostability of the variant,

optionally repeating steps b-f,

- h) selecting a variant having higher thermostability than the parent cutinase, and
- i) producing the variant to obtain the cutinase variant.
- 25. A process for enzymatic hydrolysis of a cyclic oligomer of poly(ethylene tere-5 phthalate), which process comprises treating the cyclic oligomer with a variant of a parent fungal cutinase, which variant comprises substitution of one or more amino acid residues at a position which is located:
  - within 17 Å from the location of the N-terminal amino acid (as calculated from amino acid residues in a crystal structure), and/or
  - ii) within 20 positions from the N-terminal amino acid.
  - 26. The process of the preceding claim, in which the cyclic oligomer is cyclic tri(ethylene terephthalaté).
  - 27. The process of claim 25 or 26 wherein the treatment is done at 60-75°C, preferably at 65-70°C.
- 15 28. The process of any of claims 25-27 wherein the cyclic oligomer is present in and on the fibers of a polyester containing fabric or yarn.
  - 29. The process of any of claims 25-28 which further comprises subsequently rinsing the fabric or yarn, preferably rinsing with an aqueous solution having a pH in the range of from about pH 7 to about pH 11.
- 20 30. A detergent composition comprising a surfactant and the variant of any of claims 1-18.
  - 31. A method for detecting cutinase activity in a sample, comprising incubating the sample with terephthalic acid bis(2-hydroxyethyl)ester dibenzoate and detecting hydrolysis of said ester.

Fig. 1
3D structure of cutinase from *Humicola insolens* 

|     | ATOM | 1        | N   | GLY | A | 3      | 24.424 | -7.935             | 18.390 | 1.00 | 46.73 |
|-----|------|----------|-----|-----|---|--------|--------|--------------------|--------|------|-------|
|     | ATOM | 2        | CA  | GLY | A | 3      | 23.848 | -8.994             | 17.546 |      | 42.29 |
| 5   | ATOM | 3        |     | GLY |   | 3      |        | -10.112            | 16.727 |      | 37.35 |
|     | ATOM | 4        |     | GLY |   | 3      |        | -10.913            | 16.728 |      | 35.38 |
|     | ATOM | 5        |     | ALA |   | 4      |        | -10.625            | 15.797 |      | 34.53 |
|     | ATOM | 6        |     | ALA |   | 4      |        | -10.874            | 14.555 |      | 30.95 |
|     | ATOM | 7        |     | ALA |   | 4      |        | -11.246            | 14.920 |      | 28.33 |
| 10  | ATOM | 8        | 0   | ALA |   | 4      |        | -10.499            | 14.446 |      | 22.94 |
|     | ATOM | 9        | CB  | ALA |   | 4      |        | -11.780            | 13.556 |      | 26.92 |
|     | ATOM | 10       | N   | ILE |   | 5      |        | -12.058            | 16.043 |      | 26.48 |
|     | ATOM | 11       | CA  | ILE |   | 5      |        | -12.289            | 16.637 |      | 25.65 |
|     | ATOM | 12       | C.  | ILE |   | 5      |        | -12.151            | 18.118 |      | 22.40 |
| 15  | ATOM | 13       | 0   | ILE |   | 5      |        | -12.888            | 18.717 |      | 24.74 |
|     | ATOM | 14       | CB  | ILE |   | 5      |        | -13.683            | 16.524 |      | 26.04 |
|     | ATOM | 15       |     | ILE |   | 5      |        | -13.003            | 15.050 |      | 29.85 |
|     | ATOM | 16       |     | ILE |   | 5      |        | -13.527            | 17.159 |      | 20.48 |
|     | MOTA | 17       |     | ILE |   | 5      |        | -15.133            | 14.709 |      |       |
| 20  | ATOM | 18       | N   | GLU |   | 6      |        | -13.133            |        |      | 27.96 |
| 20  | ATOM | 19       | CA  | GLU |   | 6      |        | -11.015            | 18.668 |      | 20.52 |
|     | ATOM | 20       | CA  | GLU |   | 6      |        |                    | 20.040 |      | 17.94 |
|     | ATOM |          | 0   |     |   |        |        | -11.027            | 20.432 |      | 17.76 |
|     | ATOM | 21<br>22 | CB  | GLU |   | 6      |        | -10.165<br>-9.614  | 19.990 |      | 17.60 |
| 25  | ATOM | 23       | CG  | GLU |   | 6      | 19.809 |                    | 20.199 |      | 14.22 |
| 2.5 | ATOM |          | CD  | GLU |   | 6<br>6 | 21.232 | -9.374             | 20.385 |      | 16.71 |
|     | ATOM | 24<br>25 |     | GLU |   |        |        | -10.387<br>-11.347 | 21.030 |      | 34.47 |
|     | ATOM |          | OE1 |     |   | 6      |        |                    | 21.693 |      | 49.57 |
|     | ATOM | 26       |     | GLU |   | 6      |        | -10.310            | 20.975 |      | 37.43 |
| 30  |      | 27       | N   | ASN |   | 7      |        | -11.895            | 21.333 |      | 21.67 |
| 30  | ATOM | 28       | CA  | ASN |   | 7      |        | -11.854            | 21.846 |      | 24.04 |
|     | ATOM | 29       | C   | ASN |   | 7      |        | -11.488            | 23.238 |      | 22.08 |
|     | ATOM | 30       | 0   | ASN |   | 7      |        | -12.179            | 23.820 |      | 24.00 |
|     | ATOM | 31       | CB  | ASN |   | 7      |        | -13.307            | 21.820 |      | 25.06 |
| 35  | ATOM | 32       | CG  | ASN |   | 7      |        | -13.160            | 20.341 |      | 38.52 |
| JJ  | MOTA | 33       |     | ASN |   | 7      |        |                    | 19.759 |      | 48.45 |
|     | ATOM | 34       |     | ASN |   | 7      |        | -12.081            | 19.968 |      | 36.89 |
|     | ATOM | 35       | N   | GLY |   | 8      |        | -10.813            | 23.926 |      | 23.56 |
|     | ATOM | 36       | CA  | GLY |   | 8      |        | -10.628            | 25.363 |      | 23.69 |
| 40  | ATOM | 37       | C   | GLY |   | 8      |        | -10.247            | 25.984 |      | 22.72 |
| 40  |      | 38       | 0   | GLY |   | 8      |        | -10.939            | 26.867 |      | 32.25 |
|     | ATOM | 39       | N   | LEU |   | 9      | 14.785 | ~9.144             | 25.755 |      | 23.61 |
|     | ATOM | 40       | CA  | LEU |   | 9      | 13.470 | -8.753             | 26.033 |      | 23.73 |
|     | ATOM | 41       | C   | LEU |   | 9      | 12.559 | -9.961             | 25.782 |      | 25.93 |
| 45  | ATOM | 42       | 0   | LEU |   | 9      |        | -10.054            | 26.480 |      | 30.47 |
| 45  | MOTA | 43       | CB  | LEU |   | 9      | 12.971 | -7.621             | 25.105 | 1.00 | 5.84  |
|     | MOTA | 44       | CG  | LEU |   | 9      | 11.556 |                    | 25.470 |      | 23.25 |
|     | ATOM | 45       |     | LEU |   | 9      | 11.422 |                    | 26.968 |      | 20.21 |
|     | ATOM | 46       |     | LEU |   | 9      | 11.009 |                    | 24.714 |      | 17.64 |
|     | ATOM | 47       | N   | GLU |   | 10     |        | -10.786            | 24.773 |      | 29.56 |
| 50  | MOTA | 48       | CA  | GLU |   | 10     |        | -11.681            | 24.484 | 1.00 | 33.93 |
|     | MOTA | 49       | С   | GLU | A | 10     | 11.640 | -12.872            | 25.412 | 1.00 | 32.18 |
|     | MOTA | 50       | 0   | GLU | A | 10     | 10.600 | -13.159            | 25.996 | 1.00 | 36.67 |

**ATOM** 51 CB GLU A 10 11.513 -11.996 23.012 1.00 40.97 ATOM 52 CG GLU A 10.054 -12.303 22.745 1.00 51.96 ATOM 53 CD GLU A 10 9.570 -11.711 21.437 1.00 54.08 ATOM OE1 GLU A 54 10 10.488 -11.440 20.635 1.00 48.22 ATOM 55 OE2 GLU A 8.323 -11.643 10 21.471 1.00 52.39 ATOM 56 N SER A 11 12.822 -13.334 25.688 1.00 29.58 ATOM 57 CA SER A 12.993 -14.455 26.645 11 1.00 35.25 MOTA 58 С SER A 13.403 -14.012 11 28.047 1.00 39.86 ATOM 59 0 SER A 13.688 -14.790 28.919 11 1.00 43.72 **10** ATOM CB 60 SER A 14.053 -15.364 25.983 11 1.00 33.73 ATOM 61 OG 15.275 -14.620 SER A 25.928 11 1.00 46.98 MOTA 62 N GLY A 13.467 -12.802 12 28.456 1.00 41.40 ATOM 63 CA GLY A 12 13.841 -12.332 29.752 1.00 45.34 **ATOM** 64 C GLY A 12.673 -12.562 12 30.694 1.00 47.62 15 ATOM 65 0 GLY A 12 11.485 -12.335 30.335 1.00 50.76 MOTA 66 N SER A 12.969 -12.900 31.936 13 1.00 48.09 ATOM 67 CA SER A 11.974 -13.158 32.995 13 1.00 45.26 MOTA 68 C SER A 11.509 -11.933 33.772 1.00 39.53 ATOM 69 0 SER A 13 12.563 -11.204 33.992 1.00 36.30 **20** ATOM 70 CB SER A 13 12.708 -14.006 34.101 1.00 51.20 **ATOM** 71 OG SER A 13 12.006 -13.947 35.338 1.00 57.14 MOTA 72 N ALA A 14 10.256 -11.785 34.214 1.00 35.22 ATOM 73 CA 1.00 34.78 ALA A 14 10.068 -10.530 34.964 ATOM 74 C ALA A 10.574 -10.620 36.417 14 1.00 37.51 **25** ATOM 75 O ALA A 10.809 -9.584 37.113 1.00 38.41 14 MOTA -9.915 76 CB ALA A 8.714 34.903 1.00 32.71 14 MOTA 77 N ASN A 11.039 -11.834 36.737 1.00 38.85 15 MOTA 78 CA ASN A 11.715 -12.086 37.963 15 1.00 43.49 MOTA 79 С ASN A 15 13.073 -11.411 37.953 1.00 46.45 30 ATOM 80 0 ASN A 13.453 -11.022 39.022 15 1.00 52.50 ATOM 81 CB ASN A 15 12.088 -13.533 38.207 1.00 53.08 ATOM 82 CG ASN A 10.772 -14.226 15 38.553 1.00 71.86 MOTA 83 OD1 ASN A 9.837 -13.535 1.00 71.73 15 38.998 ATOM ND2 ASN A 10.866 -15.523 84 15 38.267 1.00 77.71 35 атом 85 N ALA A 16 13.712 -11.305 36.812 1.00 46.73 ATOM 86 CA ALA A 16 14.915 -10.470 36.743 1.00 41.22 MOTA 1.00 36.70 87 C ALA A 16 15.031 -9.286 35.798 ATOM 88 0 16.027 -9.254 ALA A 16 35.075 1.00 37.67 ATOM 89 CB ALA A 15.903 -11.545 36.301 16 1.00 41.80 **40** ATOM 90 N CYS A 14.300 -8.227 17 35.843 1.00 30.62 MOTA 91 CA CYS A 17 14.614 -7.093 34.997 1.00 31.78 ATOM 92 C CYS A 16.024 -6.579 17 35.149 1.00 32.94 ATOM 1.00 39.10 93 0 CYS A 16.744 -6.850 17 36.113 ATOM 94 CB CYS A -5.881 13.679 35.138 1.00 28.00 17 45 атом 95 SG CYS A 17 12.048 -6.583 34.858 1.00 24.72 MOTA N 16.529 -5.910 96 PRO A 18 34.092 1.00 30.49 ATOM 97 CA PRO A 17.994 -5.626 33.971 1.00 22.04 18 **ATOM** 98 C 18.178 -4.138 34.241 PRO A 1.00 20.15 18 99 ATOM 0 17.085 -3.459 PRO A 18 34.370 1.00 17.83 50 атом 100 CB PRO A 18.353 -6.003 32.559 1.00 19.20 18 MOTA 101 CG PRO A 18 17.044 -6.595 32.101 1.00 20.16 CD ATOM 102 1.00 24.35 PRO A 15.903 -5.936 32.792 18 ASP A ATOM 19.428 103 N 19 -3.652 34.011 1.00 14.85

MOTA 104 CA ASP A 19 19.451 -2.168 34.226 1.00 16.59 **ATOM** 105 C ASP A 19 18.739 -1.367 33.156 1.00 20.42 106 -0.242 **ATOM** 0 ASP A 19 18.311 33.430 1.00 23.84 ATOM 107 CB ASP A 19 20.896 -1.818 34.485 1.00 27.25 5 атом 108 CG ASP A 19 21.433 -2.389 35.793 1.00 42.30 MOTA 109 OD1 ASP A 21.162 19 -3.549 36.297 1.00 53.52 OD2 ASP A ATOM 110 22.251 19 -1.719 36.543 1.00 54.02 **ATOM** 111 N ALA A 20 18.646 -1.780 31.895 1.00 20.18 MOTA 112 CA ALA A 20 18.066 -1.036 30.809 1.00 17.43 10 ATOM 113 C ALA A 20 17.713 -2.087 29.703 1.00 16.06 ATOM 114 0 ALA A 20 18.334 -3.172 29.860 1.00 9.45 ATOM 115 CB ALA A 18.975 -0.048 30.100 20 1.00 12.07 ATOM 116 N ILE A 16.814 -1.602 28.829 1.00 21 8.47 ATOM 117 CA ILE A 16.657 27.753 21 -2.583 1.00 9.23 **15 ATOM** 118 C ILE A 21 16.952 -1.745 26.486 1.00 14.77 **ATOM** 119 0 ILE A 16.681 -0.473 26.403 21 1.00 12.01 ATOM 120 CB ILE A 15.208 -2.984 27.837 1.00 16.28 21 ATOM 121 CG1 ILE A 14.851 -3.898 28.956 1.00 15.55 21 ATOM 122 CG2 ILE A 14.689 -3.671 26.514 21 1.00 13.71 20 атом 123 CD1 ILE A 21 13.401 -3.879 29.372 1.00 6.12 ATOM 124 LEU A 17.432 25.391 Ν 22 -2.451 1.00 12.24 ATOM 125 CA LEU A 17.665 -1.774 24.087 22 1.00 11.27 MOTA 126 С LEU A 23.038 22 16.849 -2.517 1.00 14.60 ATOM 127 0 LEU A 16.908 22 -3.781 22.850 1.00 9.78 25 атом 128 CB LEU A 22 19.087 -1.865 23.693 1.00 10.96 ATOM 129 CG LEU A 22 19.493 -1.543 22.257 1.00 10.32 MOTA 130 CD1 LEU A 22 19.311 -0.081 21.900 1.00 4.72 MOTA -1.842 131 CD2 LEU A 22 20.990 22.156 1.00 7.42 **ATOM** 132 N ILE A 23 16.038 -1.815 22.242 1.00 15.13 30 ATOM 133 CA ILE A 23 15.298 -2.459 21.115 1.00 18.06 MOTA 134 C ILE A 15.916 -1.771 19.901 1.00 17.42 23 MOTA 135 0 ILE A 23 16.117 -0.519 19.795 1.00 19.31 ATOM 136 CB ILE A 13.820 -2.194 21.392 23 1.00 18.16 MOTA 137 CG1 ILE A 13.208 -3.076 22.447 23 1.00 14.23 35 атом 138 CG2 ILE A 23 12.787 -2.167 20.247 1.00 13.19 MOTA CD1 ILE A -2.065 139 23 12.142 22.976 1.00 20.41 MOTA 140 N PHE A 16.218 -2.548 18.940 24 1.00 14.59 ATOM PHE A 141 CA 16.859 -2.159 17.671 24 1.00 11.72 MOTA С PHE A -2.719 142 16.347 16.353 1.00 24 7.25 40 ATOM 143 0 PHE A 24 16.095 -3.998 16.161 1.00 3.47 **ATOM** CB PHE A 18.195 -2.855 17.658 144 24 1.00 12.61 **ATOM** 145 CG PHE A 19.015 -2.150 16.716 1.00 10.72 24 MOTA CD1 PHE A 146 19.457 -0.844 16.913 1.00 13.08 24 MOTA 147 CD2 PHE A 24 19.325 -2.852 15.558 1.00 6.61 **45** атом 148 CE1 PHE A 24 20.232 -0.187 15.983 1.00 4.86 **MOTA** 20.061 1.00 149 CE2 PHE A 24 -2.218 14.545 7.61 **ATOM** 150 CZ PHE A 24 20.550 -0.823 14.804 1.00 8.78 **ATOM** 151 N ALA A 25 16.037 -1.700 15.449 1.00 ATOM 152 CA ALA A 25 15.662 -2.158 14.068 1.00 **50** ATOM 153 С ALA A 25 16.851 -1.976 13.055 1.00 1.00 ATOM 154 0 ALA A 17.518 -1.000 13.133 5.95 25 ATOM 155 CB ALA A 25 14.488 -1.402 13.562 1.00 8.27 ATOM 17.174 -3.032 156 N ARG A 26 12.325 1.00

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            158
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                              26
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5 ATOM
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                      ARG A
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   MOTA
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10 ATOM
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                      GLY A
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   MOTA
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ATOM 263 CA 25.487 LEU A 42 -0.048 19.300 1.00 12,36 MOTA 264 C LEU A 42 25.337 -0.856 20.624 1.00 11.94 MOTA 265 0 LEU A 42 25.423 -0.397 21.730 1.00 MOTA 266 CB LEU A 42 24.036 0.168 18.811 1.00 13.24 **5 ATOM** 267 CG LEU A 42 23.272 1.160 19,676 1.00 6.90 **ATOM** 268 CD1 LEU A 42 24.108 2.419 19.962 1.00 6.62 ATOM 269 ·CD2 LEU A 42 21.991 1.580 18.943 1.00 7.11 ATOM 270 N ALA A 24.905 -2.095 43 20.482 1.00 10.88 MOTA 271 CA ALA A 43 24.761 -3.027 21.553 1.00 12.37 10 атом 272 C ALA A 43 26.106 -3.136 22.252 1.00 15.45 MOTA 273 0 ALA A -2.743 25.958 23.433 43 1.00 20.80 MOTA 274 CB ALA A 43 24.148 -4.324 21.002 1.00 9:60 MOTA 275 N ASN A 27.263 -3.440 21.636 1.00 16.91 **ATOM** 276 28.454 CA ASN A 44 -3.434 22.439 1.00 20.33 **15 ATOM** 277 C ASN A 28.717 -2.044 23.113 44 1.00 17.66 278 MOTA 0 ASN A 29.019 44 -1.991 24.301 1.00 17.06 MOTA 279 CB ASN A 44 29.756 -3.695 21.625 1.00 35.48 MOTA 280 CG ASN A 44 29.564 -5.115 21.138 1.00 58.23 MOTA 281 OD1 ASN A 44 30.013 -5.403 20.034 1.00 79.77 20 MOTA 282 ND2 ASN A 44 28.908 -5.945 21.921 1.00 70.10 MOTA 283 N GLY A 45 28.682 -0.988 22.297 1.00 14.39 MOTA 284 CA GLY A 45 29.015 0.221 22.976 1.00 11.65 MOTA 285 С GLY A 45 28.175 0.255 24.234 1.00 14.30 MOTA 286 0 GLY A 45 28.529 0.582 25.385 1.00 10.77 25 атом 287 N LEU A 46 26.861 0.099 24.065 1.00 16.88 MOTA 288 CA: LEU A 46 25.968 0.248 25.207 1.00 16.29 MOTA C LEU A 289 46 26.395 -0.651 26.346 1.00 13.48 ATOM 290 0 LEU A 46 26.579 -0.325 27.462 1.00 7.75 MOTA 291 CB LEU A 46 24.608 -0.243 24.847 1.00 19.46 30 ATOM 292 CG LEU A 46 23.642 0.551 25.664 1.00 13.97 **ATOM** 293 CD1 LEU A 1.994 46 24.089 25.563 1.00 13.99 **ATOM** 294 CD2 LEU A 46 22.275 0.465 25.038 1.00 32.18 MOTA 295 N GLU A 47 26.523 -1.890 25.882 1.00 15.90 ATOM 296 CA GLU A 47 26.910 -2.886 26.909 1.00 24.03 35 атом 297 С GLU A 47 28.140 ~2.500 27.702 1.00 24.14 MOTA 298 0 GLU A 47 28.722 -3.203 28.500 1.00 27.24 ATOM 299 CB GLU A 47 27.147 -4.206 26.204 1.00 33.33 ATOM 300 CG GLU A 47 27.386 -5.254 27.245 1.00 51.29 MOTA 301 CD GLU A 47 27.661 -6.560 26.524 1.00 68.40 40 ATOM 302 OE1 GLU A 47 26.741 -7.007 25.777 1.00 66.37 ATOM 303 OE2 GLU A 28.856 -6.921 47 26.830 1.00 78.70 MOTA 304 N SER A 28.992 -1.626 48 27.215 1.00 27.50 ATOM 305 CA SER A 30.331 -1.518 48 27.789 1.00 25.23 **ATOM** 306 C SER A 30.108 -0.555 28.926 48 1.00 26.91 45 ATOM 307 O SER A 31.124 -0.058 29.462 48 1.00 33.39 ATOM 308 CB SER A 48 -0.990 26.621 31.116 1.00 21.90 MOTA 309 SER A OG 0.422 48 31.294 26.483 1.00 27.87 MOTA 310 N HIS A 28.826 -0.101 28.995 49 1.00 25.04 MOTA CA 311 HIS A 28.542 0.955 29.956 49 1.00 19.72 50 атом C 312 HIS A 49 27.480 0.461 30.950 1.00 22.55 ATOM 313 0 HIS A 49 27.186 1.089 31.898 1.00 27.93 MOTA 314 CB HIS A 28.094 2.197 49 29.463 1.00 16.13 **ATOM** 315 CG HIS A 49 28.806 3.036 28.520 1.00 39.79

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ATOM ND1 HIS A 29.564 316 49 4.058 28.953 1.00 45.66 MOTA CD2 HIS A 49 317 28.776 3.070 27.197 1.00 46.91 CE1 HIS A ATOM 318 49 30.028 4.750 27.979 1.00 45.87 **ATOM** 319 NE2 HIS A 49 29.544 4.139 26.934 1.00 50.84 **5 ATOM** 320 27.009 N ILE A 50 -0.703 30.715 1.00 18.34 MOTA 321 CA ILE A -1.129 50 25.874 31.415 1.00 19.89 **ATOM** 322 С ILE A 25.917 -2.629 50 31.146 1.00 26.29 **ATOM** 323 0 ILE 50 25.322 -3.023 30.168 1.00 25.33 **ATOM** 324 CB ILE A 50 24.527 -0.535 31.008 1.00 10.50 **10** ATOM CG1 ILE A 325 50 24.340 0.906 31.292 1.00 4.97 CG2 ILE A ATOM 326 50 23.466 -1.298 31.697 1.00 12.96 ATOM 327 CD1 ILE A 50 23.413 1.845 30.602 1.00 16.65 ATOM 328 N ARG A 51 26.707 -3.256 32.066 1.00 31.77 **ATOM** 329 CA ARG A 51 26.887 -4.714 32.107 1.00 29.06 **15 ATOM** 330 C ARG A 25.457 -5.331 32.170 51 1.00 32.68 ATOM 331 0 ARG A 51 25.396 -6.363 31.512 1.00 37.16 ATOM 332 N ASN A 52 24.380 -4.817 32.788 1.00 28.48 MOTA 333 CA ASN A 52 23.284 -5.767 32.832 1.00 26.39 MOTA 334 С ASN A 52 22.176 -5.178 31.993 1.00 27.75 20 атом 335 0 ASN A 52 21.333 -4.488 32.636 1.00 26.68 ATOM 336 CB ASN A 52 22.750 -5.884 34.232 1.00 34.86 ATOM 337 CG ASN A 52 21.637 -6.879 34.271 1.00 39.54 ATOM 338 20.781 OD1 ASN A 52 -6.541 35.095 1.00 54.31 ATOM 339 ND2 ASN A 21.611 -7.954 33.503 52 1.00 48.82 25 атом 340 22.127 N ILE A 53 -5.699 30.800 1.00 24.42 ATOM 341 CA ILE A 21.261 29.772 53 -5.092 1.00 20.15 MOTA 342 С ILE A 53 20.585 -6.151 28.912 1.00 17.63 MOTA 343 0 ILE A 21.020 -7.349 28.917 53 1.00 18.01 ATOM 344 CB ILE A 53 22.245 -4.297 28.880 1.00 14.09 30 ATOM CG1 ILE A 345 21.682 53 -3.257 27.936 1.00 22.91 MOTA 346 CG2 ILE A 22.907 27.946 53 -5.321 1.00 16.37 MOTA 347 CD1 ILE A 22.877 -2.315 27.622 53 1.00 38.17 **ATOM** 348 N TRP A 54 19.447 -5.880 28.383 1.00 15.19 MOTA 349 CA TRP A 18.804 -6.889 27.567 54 1.00 17.96 **35** ATOM 350 C TRP A 54 18.803 -6.230 26.151 1.00 19.82 MOTA 351 0 TRP A 54 18.340 -5.059 25.985 1.00 18.37 ATOM 352 CB TRP A 17.364 -7.046 27.998 54 1.00 23.18 ATOM 353 CG TRP A 54 16.949 -7.932 29.100 1.00 24.57 ATOM 354 CD1 TRP A 54 17.757 -8.727 29.895 1.00 24.46 40 ATOM 355 CD2 TRP A 54 15.595 -8.164 29.603 1.00 30.21 ATOM 356 NE1 TRP A 17.004 -9.372 30.858 1.00 25.87 54 MOTA 357 CE2 TRP A 15.692 -9.039 30.700 54 1.00 24.92 ATOM 358 CE3 TRP A 14.358 -7.633 29.243 54 1.00 36.26 MOTA 359 CZ2 TRP A 14.611 -9.442 31.432 1.00 19.75 54 **45** ATOM 360 CZ3 TRP A 13.316 -8.042 30.009 1.00 32.94 54 ATOM 361 CH2 TRP A -8.916 31.068 54 13.451 1.00 23.02 ATOM 362 ILE A -7.152 25.204 Ν 55 19.063 1.00 15.21 MOTA 363 CA ILE A 55 19.178 -6.655 23.838 1.00 12.41 ATOM 364 С ILE A 55 18.091 -7.215 22.962 1.00 11.40 50 ATOM 365 17.955 22.680 1.00 7.34 0 ILE A 55 -8.378 **ATOM** 366 CB ILE A 55 20.546 -6.962 23.201 1.00 16.44 ATOM 23.702 367 CG1 ILE A 55 21.939 -6.409 1.00 8.75 ATOM 368 20.384 -6.460 21.750 1.00 21.77 CG2 ILE A 55

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ATOM
            369
                  CD1 ILE A
                              55
                                       21.767
                                                -5.582
                                                         24.863
                                                                  1.00 16.23
   MOTA
            370
                 N
                      GLN A
                              56
                                       17.226
                                                                  1.00 9.67
                                                -6.412
                                                         22.390
   ATOM
            371
                 CA
                      GLN A
                              56
                                       16.161
                                                -7.016
                                                        21.619
                                                                  1.00 10.90
   MOTA
            372
                 C
                      GLN A
                              56
                                       16.432
                                                -6.621
                                                        20.143
                                                                  1.00 13.08
 5 ATOM
            373
                 0
                      GLN A
                              56
                                       16.402
                                                -5.393
                                                         19.953
                                                                  1.00 10.32
   MOTA
            374
                 CB
                      GLN A
                              56
                                       14.786
                                                -6.542
                                                         22.014
                                                                  1.00 11.49
   MOTA
            375
                 CG
                      GLN A
                              56
                                       13.653
                                                -7.256
                                                         21,316
                                                                  1.00 23.47
   ATOM
            376
                  CD
                      GLN A
                              56
                                       13.789
                                                -8.741
                                                         21.351
                                                                  1.00 24.88
   ATOM
            377
                 OE1 GLN A
                              56
                                       13.610
                                                -9.379
                                                         20.324
                                                                  1.00
                                                                       9.56
10 атом
            378
                 NE2 GLN A
                              56
                                       14.119
                                                -9.221
                                                         22.544
                                                                  1.00 17.94
   ATOM
            379
                 N
                      GLY A
                              57
                                       16.288
                                                -7.645
                                                         19.216
                                                                  1.00
                                                                       6.84
   ATOM
            380
                 CA
                      GLY A
                              57
                                       16.174
                                                -7.019
                                                         17.841
                                                                  1.00 16.15
   ATOM
            381
                 С
                      GLY A
                              57
                                       14.740
                                                -7.085
                                                         17.267
                                                                  1.00 13.72
   ATOM
            382
                 0
                      GLY A
                                                         17.752
                                       14.124
                                                -8.016
                                                                  1.00 12.70
15 ATOM
            383
                 N
                      VAL A
                              58
                                       14.068
                                                -6.264
                                                         16.525
                                                                  1.00 12.73
   ATOM
            384
                 CA
                      VAL A
                              58
                                       12.739
                                                -6.308
                                                         16.070
                                                                  1.00 11.16
   ATOM
            385
                 С
                      VAL A
                              58
                                       12.715
                                                -7.246
                                                        14.893
                                                                  1.00 14.85
   ATOM
            386
                 0
                      VAL A
                              58
                                       13.234
                                                -6.891
                                                        13.849
                                                                  1.00 18.64
   ATOM
            387
                 CB
                      VAL A
                              58
                                       12.262
                                                -4.984
                                                        15.352
                                                                  1.00
                                                                        6.54
20 атом
            388
                  CG1 VAL A
                              58
                                       10.894
                                                -4.974
                                                         14.731
                                                                  1.00
   ATOM
            389
                  CG2 VAL A
                              58
                                       12.650
                                                -3.840
                                                         16.331
                                                                  1.00 5.86
   ATOM
            390
                 N
                      GLY A
                              59
                                       12.209
                                                -8.465
                                                         15.008
                                                                  1.00 21.96
   ATOM
            391
                  CA
                      GLY A
                              59
                                       12.120
                                                -9.385
                                                        13.874
                                                                  1.00 17.81
   ATOM
            392
                  C
                      GLY A
                              59
                                       10.645
                                                -9.561
                                                         13.550
                                                                  1.00 23.35
25 атом
            393
                  0
                      GLY A
                              59
                                        9.919
                                                -8.579
                                                         13.249
                                                                  1.00 27.99
   ATOM
            394
                 N
                      GLY A
                              60
                                       10.166 -10.805
                                                         13.623
                                                                  1.00 18.75
   ATOM
            395
                 CA
                      GLY A
                              60
                                        8.841 -11.142
                                                                  1.00 11.46
                                                         13.285
   ATOM
            396
                  C
                      GLY A
                                        8.550 -10.833
                              60
                                                         11.851
                                                                  1.00 14.56
   ATOM
            397
                  0
                      GLY A
                              60
                                        9.160 -11.439
                                                         11.003
                                                                  1.00 16.32
30 ATOM
            398
                 N
                      PRO A
                                        7.505 -10.103
                              61
                                                         11.612
                                                                  1.00 12.10
   ATOM
            399
                  CA
                      PRO A
                              61
                                        7.123
                                                -9.774
                                                         10.250
                                                                  1.00 14.70
   ATOM
            400
                  С
                      PRO A
                                        8.230
                              61
                                                -8.941
                                                          9.570
                                                                  1.00 22.17
   ATOM
            401
                  0
                      PRO A
                                        8.143
                                                -8.758
                                                          8.344
                                                                  1.00 25.74
   ATOM
            402
                  CB
                      PRO A
                              61
                                        5.911
                                                -8.860
                                                         10.332
                                                                  1.00 14.30
35 атом
            403
                  CG
                      PRO A
                              61
                                        5.880
                                                -8.514
                                                         11.784
                                                                  1.00 13.62
   MOTA
            404
                  CD
                      PRO A
                                        6.723
                              61
                                                -9.417
                                                         12.576
                                                                  1.00 12.29
            405
   ATOM
                 N
                      TYR A
                              62
                                        9.162
                                                -8.257
                                                         10.292
                                                                  1.00 21.56
   ATOM
            406
                  CA
                      TYR A
                              62
                                        9.973
                                                -7.242
                                                          9.674
                                                                  1.00 17.07
   ATOM
            407
                  C
                      TYR A
                              62
                                       11.133
                                                -7.907
                                                          9.047
                                                                  1.00 18.73
40 ATOM
            408
                 0
                      TYR A
                              62
                                       12.132
                                                -8.213
                                                          9.691
                                                                  1.00 22.39
   ATOM
            409
                 CB
                      TYR A
                              62
                                       10.504
                                                -6.401
                                                        10.803
                                                                  1.00 17.51
   MOTA
            410
                  CG
                      TYR A
                              62
                                       11.461
                                                -5.421
                                                         10.236
                                                                  1.00 15.23
   ATOM
                  CD1 TYR A
            411
                              62
                                       11.343
                                                -4.920
                                                          9.032
                                                                  1.00 17.79
   ATOM
            412
                  CD2 TYR A
                              62
                                       12.465
                                                -4.971
                                                         10.969
                                                                  1.00 19.09
45 ATOM
            413
                 CE1 TYR A
                              62
                                       12.206
                                                -3.997
                                                          8.506
                                                                  1.00 19.28
   ATOM
                  CE2 TYR A
            414
                              62
                                       13.438
                                                -4.101
                                                        10.490
                                                                  1.00 25.40
   ATOM
            415
                  CZ
                      TYR A
                              62
                                       13.327
                                                -3.571
                                                          9.186
                                                                  1.00 20.95
   ATOM
            416
                  OH
                      TYR A
                              62
                                       14.320
                                                -2.649
                                                          8.791
                                                                  1.00 14.70
   MOTA
            417
                 N
                      ASP A
                                       10.998
                              63
                                                -8.419
                                                          7.816
                                                                  1.00 19.47
50 ATOM
            418
                  CA
                      ASP A
                                       12.137
                                                -9.011
                                                          7.081
                                                                  1.00 17.52
   ATOM
            419
                  C
                      ASP A
                              63
                                       13.027
                                                -7.973
                                                          6.453
                                                                  1.00 17.97
   MOTA
            420
                  0
                      ASP A
                              63
                                       13.628
                                                -8.442
                                                          5.512
                                                                  1.00 14.94
   ATOM
            421
                  CB
                      ASP A
                              63
                                       11.474
                                                -9.873
                                                          6.015
                                                                  1.00 17.16
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MOTA 422 CG ASP A 63 10.563 -9.136 5.096 1.00 27.75 **ATOM** 423 OD1 ASP A 63 10.049 -8.030 5.281 1.00 34.11 ATOM 424 OD2 ASP A 63 10.300 -9.635 4.002 1.00 44.13 ATOM 425 N ALA A 13.089 64 -6.685 6.584 1.00 15.36 5 атом 426 CA ALA A 64 14.054 -5.725 6.098 1.00 17.14 ATOM 427 C ALA A 64 14.118 -5.780 4.589 1.00 21.10 MOTA 428 0 ALA A 64 15.193 -5.861 3.968 1.00 23.12 ATOM 429 CB ALA A 15.458 64 -5.861 6.646 1.00 20.45 ATOM 430 N ALA A 65 12.946 -6.009 4.006 1.00 22.21 **10 ATOM** 431 CA ALA A -6.072 65 12.817 2.565 1.00 21.81 ATOM 432 C ALA A -4.857 65 13.143 1.745 1.00 21.76 **ATOM** 433 0 ALA A 12.855 65 -3.801 2.229 1.00 23.60 ATOM 434 CB ALA A 65 11.384 -6.390 2.364 1.00 17.31 ATOM 435 N LEU A 66 13.401 -4.866 0.402 1.00 21.48 **15** ATOM 436 CA LEU A 13.763 66 -3.581 -0.216 1.00 13.20 **ATOM** 437 C LEU A 12.469 66 -2.913 -0.452 1.00 13.90 MOTA 438 0 LEU A 66 12.548 -1.767 -0.197 1.00 11.85 **ATOM** 439 CB LEU A 66 14.593 -3.602 -1.470 1.00 3.92 **ATOM** 440 CG LEU A 66 15.891 -4.308 -1.191 1.00 9.05 20 ATOM 441 CD1 LEU A 66 16.509 -4.725 -2.438 1.00 12.78 ATOM 442 CD2 LEU A 66 16.569 -3.119 -0.580 1.00 13.44 ATOM 443 N ALA A 67 11.413 -3.625 -0.801 1.00 14.94 **ATOM** 444 CA -1.277 ALA A 67 10.253 -2.759 1.00 12.42 MOTA 445 C ALA A 67 9.626 -1.879 -0.224 1.00 14.21 25 атом 446 0 ALA A 67 9.218 -0.818 -0.643 1.00 14.29 **ATOM** 447 CB ALA A 67 9.089 -3.588 -1.781 1.00 3.90 ATOM 448 N THR A 68 1 9.494 -2.409 1.006 1.00 12.11 MOTA 449 CA THR A 8.780 68 -1.647 1.997 1.00 11.77 **ATOM** 450 C THR A 9.242 68 -0.214 2.219 1.00 13.05 30 ATOM 451 0 THR A 68 8.597 0.683 2.766 1.00 11.13 MOTA 452 CB THR A 8.892 68 -2.488 3.241 1.00 13.93 **ATOM** 453 OG1 THR A 68 10.145 -3.150 3.224 1.00 27.44 ATOM 454 CG2 THR A 7.783 68 -3.459 3.087 1.00 13.39 MOTA 455 N ASN A 69 10.450 -0.057 1.808 1.00 7.59 35 ATOM 456 CA ASN A 69 11.020 1.236 1.791 1.00 8.76 MOTA 457 C ASN A 69 10.095 2.165 1.047 1.00 10.28 ATOM 458 0 ASN A 69 9.950 3.345 1.305 1.00 5.30 **ATOM** 459 CB ASN A 69 12.461 1.251 1.231 1.00 5.54 ATOM 460 CG ASN A 69 13.374 1.207 2.398 1.00 15.08 **40** ATOM 461 OD1 ASN A 69 13.307 2.124 3.275 1.00 31.90 ATOM 462 ND2 ASN A 69 14.048 0.099 2.360 1.00 4.51 ATOM 463 N PHE A 70 9.390 1.656 1.00 19.09 0.079 MOTA 464 CA PHE A 70 8.552 2.619 -0.631 1.00 21.80 MOTA 465 C PHE A 70 7.157 2.836 -0.123 1.00 23.36 **45** ATOM 466 PHE A 0 70 6.509 3.717 -0.724 1.00 25.74 ATOM 467 CB PHE A 70 8.547 2.386 -2.082 1.00 17.38 MOTA 468 CG PHE A 70 9.870 2.360 -2.770 1.00 15.72 ATOM 469 CD1 PHE A 10.080 70 3.430 -3.576 1.00 5.15 MOTA 470 CD2 PHE A 70 10.702 1.245 -2.497 1.00 7.61 50 атом 471 CE1 PHE A 70 11.268 3.330 -4.191 1.00 16.05 MOTA 472 CE2 PHE A 70 11.913 1.267 -3.168 1.00 22.23 ATOM 473 CZPHE A 70 12.199 2.314 -4.016 1.00 9.57 MOTA 474 N LEU A 71 6.765 2.246 1.034 1.00 25.53

475 MOTA CA LEU A 71 5.506 2.725 1.599 1.00 24.24 ATOM 476 C LEU A 71 5.649 4.037 2.343 1.00 27.91 ATOM 477 0 LEU A 71 6.694 4.521 2.750 1.00 28.86 ATOM 478 CB LEU A 71 5.150 1.635 2.535 1.00 19.99 **5 ATOM** 479 CG LEU A 71 5.003 0.342 1.873 1.00 16.09 **ATOM** 480 CD1 LEU A 71 4.879 -0.764 2.885 1.00 18.12 **ATOM** 481 CD2 LEU A 71 3.786 0.546 1.000 1.00 18.24 **ATOM** 482 N PRO A 72 4.535 4.663 2.529 1.00 33.01 ATOM 483 CA PRO A 72 4.389 5.888 3.311 1.00 34.96 10 ATOM 484 C PRO A 72 4.865 5.590 4.778 1.00 32.90 MOTA 485 0 PRO A 72 4.619 4.512 5.331 1.00 28.55 MOTA 486 CB PRO A 72 2.983 6.453 3.095 1.00 32.98 MOTA 487 CG PRO A 72 2.224 5.189 2.827 1.00 30.36 ATOM 488 CD PRO A 72 3.188 4.093 2.380 1.00 33.56 **15 ATOM** 489 N ARG A 73 5.601 6.610 5.221 1.00 27.54 MOTA 490 CA ARG A 73 6.325 6.547 6.408 1.00 25.42 MOTA 491 C ARG A 73 7.613 5.755 6.321 1.00 21.78 ATOM 492 0 ARG A 73 8.360 5.950 7.304 1.00 29.61 **ATOM** 493 CB ARG A 73 5.469 7.549 5.978 1.00 24.29 20 атом 494 CG ARG A 73 4.575 6.998 8.155 1.00 23.47 **ATOM** 495 CD ARG A 73 3.818 6.793 9.360 1.00 29.73 MOTA 496 NE ARG A 73 3.222 5.460 9.392 1.00 36.30 ATOM 497 CZARG A 73 2.891 5.312 10.713 1.00 42.26 MOTA 498 NH1 ARG A 73 3.145 6.288 11.555 1.00 26.57 **25** ATOM NH2 ARG A 499 73 2.320 4.144 10.883 1.00 39.03 ATOM 500 N GLY A 74 7.868 4.909 5.326 1.00 8.42 ATOM 501 CA GLY A 74 9.120 4.291 5.332 1.00 5.06 MOTA 502 С GLY A 9.243 2.858 5.508 1.00 12.74 MOTA 503 0 GLY A 74 10.256 2.286 5.317 1.00 16.46 30 атом 504 N THR A 75 8.145 2.321 5.906 1.00 12.82 MOTA 505 CA THR A 75 8.036 0.869 6.008 1.00 11.14 ATOM 506 C THR A 75 6.625 1.00 10.64 0.428 6.134 ATOM 507 0 THR A 75 5.757 5.949 1.231 1.00 9.36 **ATOM** 508 CB THR A 75 8.843 0.398 7.219 1.00 6.97 35 ATOM 509 OG1 THR A 75 8.938 -0.950 7.125 1.00 5.64 ATOM 510 CG2 THR A 75 8.108 0.865 8.603 1.00 6.30 MOTA 511 N SER A 76 6.409 -0.858 6.259 1.00 10.07 MOTA 512 CA SER A 76 5.061 -1.384 6.354 1.00 13.33 MOTA 513 C SER A 76 4.405 -1.163 7.747 1.00 21.87 40 атом 514 0 SER A 76 5.228 -1.102 8.679 1.00 24.22 ATOM 515 CB SER A 76 5.030 -2.832 6.083 1.00 4.81 MOTA 516 OG SER A -3.664 76 5.327 7.107 1.00 16.98 MOTA 517 N GLN A 77 3.082 -1.100 7.911 1.00 24.90 MOTA 518 CA GLN A 77 2.454 -1.020 9.166 1.00 23.85 45 атом 519 С GLN A 77 2.643 -2.236 10.015 1.00 19.58 **ATOM** 520 0 GLN A 77 2.908 -2.140 11.203 1.00 15.15 **ATOM** 521 CB GLN A 77 0.983 -0.703 9.217 1.00 32.64 **ATOM** 522 CG GLN A 77 0.567 -0.580 10.642 1.00 49.56 MOTA 523 CD GLN A 77 0.689 0.785 11.194 1.00 65.91 **50 ATOM** 524 OE1 GLN A 77 0.956 0.869 1.00 66.06 12.356 ATOM 525 NE2 GLN A 77 0.481 1.750 10.350 1.00 68.91 MOTA 526 N ALA A 78 2.754 -3.376 9.402 1.00 15.90 ATOM 527 CA ALA A 78 3.071 -4.577 10.073 1.00 19.47

MOTA 528 C ALA A 78 4.381 -4.332 10.819 1.00 24.48 MOTA 529 0 ALA A 78 4.389 -4.729 11.983 1.00 26.91 MOTA 78 530 CB ALA A 3.390 -5.808 9.336 1.00 17.23 ATOM 531 N ASN A 79 5.350 -3.863 10.093 1.00 21.58 5 атом 532 CA ASN A 79 6.602 -3.576 10.774 1.00 20.62 MOTA 533 C ASN A 79 6.480 -2.673 11.969 1.00 20.93 ATOM 534 0 ASN A 6.975 -2.944 79 13.053 1.00 15.52 **ATOM** 535 CB ASN A 79 7.474 -3.069 9.670 1.00 24.79 ATOM 536 CG ASN A 79 7.933 -4.238 8.824 1.00 28.76 10 атом 537 OD1 ASN A 7.867 9.091 79 -5.439 1.00 25.30 MOTA 538 ND2 ASN A 79 8.488 -3.891 7.660 1.00 24.90 ATOM 539 N ILE A 80 5.731 -1.611 11.936 1.00 15.93 ATOM 540 CA ILE A 80 5.586 -0.574 12.924 1.00 17.00 MOTA 541 C ILE A 4.925 80 -1.187 14.118 1.00 20.63 **15** атом 542 0 ILE A 80 5.234 -0.939 15.264 1.00 18.79 MOTA 543 CB ILE A 4.756 80 0.629 12.436 1.00 11.98 ATOM 544 CG1 ILE A 5.627 80 1.124 11.297 1.00 ATOM 545 CG2 ILE A 80 4.379 1.728 13.354 1.00 16.27 ATOM 546 CD1 ILE A 80 5.007 2.071 10.424 1.00 8.15 20 ATOM 547 N ASP A 81 4.017 -2.019 13.708 1.00 19.21 ATOM CA 548 ASP A 3.304 -2.778 81 14.728 1.00 15.15 MOTA 549 С ASP A 81 4.147 -3.711 15.510 1.00 15.77 ATOM 550 0 ASP 4.084 -3.697 Α 81 16.695 1.00 15.82 MOTA 551 ASP A CB 81 2.291 -3.438 13.868 1.00 26.36 25 атом 552 CG ASP A 1.065 -2.530 81 13.790 1.00 23.71 ATOM 553 OD1 ASP A 1.105 -1.355 14.226 81 1.00 14.33 OD2 ASP A MOTA 554 0.061 -3.125 13.222 1.00 33.05 81 ATOM 555 N GLU A 82 5.148 -4.447 15.096 1.00 16.07 MOTA 556 CA GLU A 82 5.984 -5.318 15.882 1.00 14.77 30 атом 557 C GLU A 82 6.839 -4.355 16.667 1.00 19.33 ATOM 558 0 GLU A 82 7.315 -4.708 17.752 1.00 23.58 ATOM 559 -6.031 CB GLU A 82 6.998 15.064 1.00 13.20 ATOM 560 CG 7.792 GLU A 82 -7.239 15.476 1.00 23.09 MOTA 561 CD GLU A 82 6.767 -8.114 16.185 1.00 29.68 35 атом 562 OE1 GLU A 5.666 -7.670 16.403 82 1.00 26.63 **ATOM** 563 GLU A OE2 82 7.273 -9.181 16.411 1.00 33.08 ATOM 564 N GLY A 7.228 -3.227 16.199 83 1.00 16.79 MOTA 565 CA GLY A 8.033 -2.428 83 17.140 1.00 17.32 ATOM 566 C GLY A 7.238 ~2.018 18.366 83 1.00 17.54 40 ATOM 567 0 GLY A 83 7.561 -2.103 19.528 1.00 15.06 **ATOM** 568 N LYS A 84 6.093 -1.408 18.114 1.00 18.72 MOTA 5.050 569 CA LYS A 84 -1.146 19.096 1.00 16.90 **ATOM** 570 C LYS A 4.893 -2.337 20.057 84 1.00 17.74 MOTA 571 0 LYS A 84 4.962 -2.265 21.295 1.00 14.31 45 атом 572 CB LYS A 3.799 -0.872 18.307 84 1.00 14.62 MOTA 573 1.00 19.30 CG LYS A 84 3.535 0.565 18.291 **ATOM** 574 CD LYS A 2.787 1.013 84 17.044 1.00 34.24 MOTA 575 CE LYS A 84 1.568 1.902 17.337 1.00 37.70 MOTA 576 NZ LYS A 84 0.346 1.226 16.827 1.00 48.42 **50** ATOM 577 N ARG A 85 4.617 -3.506 19.519 1.00 18.50 MOTA 578 CA ARG A 85 4.583 -4.705 20.280 1.00 19.04 MOTA 579 C ARG A 85 5.677 -4.733 21.308 1.00 19.63 ATOM 580 0 ARG A 85 5.442 -5.192 22.383 1.00 19.24

CB ARG A 85 4.740 -5.979 19.464 ATOM 581 1.00 14.74 -7.094 1.00 ATOM 582 CG ARG A 85 3.843 19.887 8.85 ATOM 583 CD ARG A 85 4.146 -8.554 19.705 1.00 7.20 MOTA 584 5.483 -8.898 NE ARG A 85 19.194 1.00 20.30 5 атом 585 CZARG A 85 6.170 -9.705 19.899 1.00 18.19 5.627 -10.161 21.040 ATOM 586 NH1 ARG A 85 1.00 34.03 7.345 -9.979 19.555 MOTA 587 NH2 ARG A 1.00 15.36 85 MOTA 588 N LEU A 86 6.901 -4.586 20.956 1.00 22.21 8.006 ATOM 589 CA LEU A 86 -4.792 21.873 1.00 20.94 С 8.044 **10** ATOM 590 -3.637 22.803 1.00 20.73 LEU A 86 591 8.155 -3.970 23.925 MOTA 0 LEU A 86 1.00 22.18 MOTA 592 CB LEU A 86 9.333 -4.932 21.168 1.00 6.67 MOTA 9.358 -6.241 20.282 593 CG LEU A 86 1.00 11.45 CD1 LEU A MOTA 594 86 10.546 -6.054 19.287 1.00 18.60 **15** атом 9.362 595 CD2 LEU A -7.516 21.020 1.00 5.17 86 7.700 MOTA 596 -2.446 22.529 1.00 16.79 N PHE A 87 7.850 MOTA 597 CA PHE A 87 -1.416 23.492 1.00 18.21 6.939 -1.805 24.618 1.00 26.51 **ATOM** 598 C PHE A 87 MOTA 599 7.082 -1.565 25.839 1.00 30.36 0 PHE A 87 20 атом 7.498 22.846 1.00 15.81 600 CB PHE A -0.118 87 8.661 0.503 22.128 MOTA 601 CG PHE A 87 1.00 22.72 ATOM 602 CD1 PHE A 87 9.625 1.163 22.795 1.00 25.90 ATOM 603 CD2 PHE A 87 8.800 0.446 20.774 1.00 24.19 10.699 1.781 22.220 **ATOM** 604 CE1 PHE A 87 1.00 26.46 25 атом 605 CE2 PHE A 9.871 0.991 20.153 1.00 29.24 87 10.827 1.669 20.849 1.00 20.81 MOTA 606 CZPHE A 87 5.862 -2.422 24.266 1.00 29.15 ATOM 607 N ALA A 88 4.772 -2.699 25.195 ATOM 1.00 22.92 608 CA ALA A 88 -3.837 26.068 ATOM 609 С ALA A 88 5.186 1.00 22.03 30 ATOM ALA A 4.974 -3.879 27.284 1.00 27.02 610 0 88 3.551 24.299 MOTA 611 CB ALA A -2.803 1.00 22.13 88 MOTA LEU A 5.649 -4.897 25.531 1.00 19.16 612 N 89 ATOM CA LEU A 6.188 -6.032 26.208 1.00 19.29 613 89 **ATOM** C LEU A 7.250 -5.507 27.133 1.00 22.06 614 89 35 ATOM 615 0 LEU A 89 7.449 -6.050 28.177 1.00 20.49 ATOM 616 CB LEU A 89 7.021 -6.863 25.221 1.00 18.41 **ATOM** 617 CG LEU A 89 7.477 -8.167 25.834 1.00 20.45 6.326 -8.707 26.627 1.00 17.22 **ATOM** 618 CD1 LEU A 89 8.060 -9.057 24.769 1.00 18.83 MOTA 619 CD2 LEU A 89 40 ATOM 8.124 -4.644 26.722 1.00 22.80 620 N ALA A 90 27.701 MOTA 621 CA ALA A 90 9.027 -4.137 1.00 24.14 MOTA 8.237 -3.488 28.849 1.00 23.63 622 С ALA A 90 ALA A MOTA 623 0 8.414 -3.835 30.071 1.00 22.73 90 27.139 1.00 7.74 MOTA 10.080 -3.253 624 CB ALA A 90 45 ATOM 1.00 25.45 -2.445 28.732 625 N ASN A 91 7.457 **ATOM** CA 6.665 -1.979 29.870 1.00 27.25 626 ASN A 91 -2.996 1.00 30.97 ATOM 627 ASN A 91 5.847 30.656 C 5.346 -2.884 31.768 1.00 27.64 ATOM 628 0 ASN A 91 29.125 5.560 -1.206 1.00 29.14 ATOM 629 CB ASN A 91 **50** ATOM -0.345 30.216 1.00 31.73 ASN A 4.946 630 CG 91 3.845 -0.692 30.645 1.00 46.76 ATOM 631 OD1 ASN A 91 1.00 29.03 5.641 0.629 30.643 **ATOM** ND2 ASN A 632 91 -4.008 29.969 1.00 35.37 5.369 MOTA 633 N GLN A 92

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634 CA GLN A 92 4.702 -5.141 30.591 1.00 35.55 MOTA MOTA 635 С GLN A 92 5.619 -6.072 31.352 1.00 34.28 ATOM 636 0 GLN A 92 5.227 -6.519 32.440 1.00 39.47 ATOM GLN A 3.866 -5.903 29.573 637 CB 92 1.00 54.94 5 атом 638 CG GLN A 2.689 -6.698 30.142 92 1.00 78.63 -8.167 ATOM 639 CD GLN A 2.806 29.805 92 1.00 93.87 ATOM 640 OE1 GLN A 3.597 -8.840 30.475 92 1.00 96.99 ATOM 641 NE2 GLN A 92 2.083 -8.696 28.824 1.00 97.81 6.859 ATOM 642 N LYS A 93 -6.403 31.050 1.00 31.97 -7.204 **10** ATOM 643 7.675 CA LYS A 93 31.972 1.00 25.22 8.381 **ATOM** 644 С LYS A 93 -6.298 33.015 1.00 24.68 ATOM 645 0 LYS A 93 8.716 -6.793 34.075 1.00 32.13 MOTA 646 CB LYS A 93 8.673 -7.980 31.148 1.00 10.86 ATOM 647 CG LYS A 8.225 -8.963 30.159 93 1.00 24.26 15 ATOM 648 CD LYS A 9.362 -9.966 29.986 93 1.00 21.96 ATOM 649 CE LYS A 93 9.093 -10.718 28.658 1.00 23.78 MOTA 10.084 -11.805 650 ΝZ LYS A 93 28.300 1.00 25.87 MOTA 651 CYS A 8.752 -5.096 32.774 N 1.00 16.62 94 MOTA 9.752 -4.412 33.480 652 CA CYS A 1.00 18.95 94 20 атом 9.512 -2.936 33.537 653 С CYS A 94 1.00 24.83 ATOM 654 CYS A 10.184 -2.017 33.150 1.00 26.80 0 94 MOTA 655 CB CYS A 11.147 -4.691 32.911 1.00 3.14 94 ATOM 656 CYS A 11.618 -6.437 32.882 1.00 25.28 SG 94 MOTA 657 N PRO A 8.403 -2.561 34.086 1.00 26.08 95 25 атом 658 CA PRO A 95 7.891 -1.202 33.878 1.00 26.11 MOTA 659 C PRO A 95 8.960 -0.259 34.299 1.00 27.32 MOTA 660 8.776 0 PRO A 95 0.966 34.108 1.00 29.08 MOTA 661 CB PRO A 6.609 ~1.090 34.747 1.00 20.75 95 ATOM 662 CG PRO A 6.587 -2.421 35.322 1.00 19.04 95 30 атом 663 CD 7.363 -3.461 34.509 1.00 22.55 PRO A 95 ATOM 664 N ASN A 96 9.836 -0.776 35.193 1.00 31.44 ATOM 665 ASN A 10.559 0.274 35.966 1.00 35.38 CA 96 **ATOM** 666 C ASN A 96 11.891 0.476 35.353 1.00 33.83 MOTA 667 12.599 1.359 0 ASN A 35.684 1.00 33.31 96 35 ATOM 668 ASN A 10.558 -0.099 37.429 CB 96 1.00 53.70 MOTA 669 CG ASN A 96 9.238 0.342 38.026 1.00 61.69 MOTA 670 OD1 ASN A 8.758 1.432 37.706 96 1.00 64.33 MOTA 671 ND2 ASN A 96 8.676 -0.526 38.861 1.00 67.25 MOTA 672 THR A 12.287 -0.409 34.507 N 97 1.00 30.32 40 ATOM 673 CA THR A 13.519 -0.367 33.794 1.00 22.83 97 **ATOM** 674 С THR A 13.404 0.493 32.534 1.00 22.44 97 MOTA 675 0 THR A 12.446 0.779 31.816 1.00 21.14 97 MOTA 676 CB THR A 97 13.835 -1.851 33.705 1.00 25.87 MOTA 677 OG1 THR A -1.915 32.528 1.00 38.91 97 14.602 45 атом 678 -2.901 33.621 1.00 24.22 CG2 THR A 97 12.769 MOTA 679 N PRO A 14.393 1.415 32.408 1.00 20.59 98 ATOM 680 CA PRO A 14.513 2.292 31.254 1.00 18.15 98 ATOM 681 С 14.882 1.494 29.978 1.00 16.07 PRO A 98 **ATOM** 15.622 0.462 1.00 17.19 682 0 PRO A 98 29.934 50 атом 683 CB PRO A 15.563 3.339 31.676 1.00 14.55 98 **ATOM** 684 CG PRO A 16.270 2.646 32.699 1.00 12.29 98 MOTA 685 CD PRO A 98 15.735 1.331 33.046 1.00 12.02 MOTA 686 N VAL A 99 14.322 2.107 28.940 1.00 13.81

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ATOM 687 VAL A CA 99 14.225 1.544 27.632 1.00 14.02 ATOM 688 C VAL A 99 14.956 2.407 26.663 1.00 10.66 **ATOM** VAL A 689 0 99 14.716 3.679 26.712 1.00 6.90 MOTA 690 CB VAL A 99 12.673 1.343 27.335 1.00 2.87 5 ATOM CG1 VAL A 691 99 12.666 1.272 25.872 1.00 17.40 ATOM 692 CG2 VAL A 99 12.442 -0.111 27.744 1.00 5.75 MOTA 1.776 693 N VAL A 100 15.885 25.861 1.00 6.45 MOTA 694 CA VAL A 100 16.525 2.755 24.900 1.00 9.61 MOTA 695 C VAL A 100 16.389 2.159 23.561 1.00 10.79 **10 ATOM** 696 **VAL A 100** 0 16.256 0.973 23.477 1.00 9.11 **ATOM** 697 CB **VAL A 100** 17.877 3.260 25.197 1.00 8.05 ATOM 698 CG1 VAL A 100 17.824 4.252 26.336 1.00 6.05 MOTA 699 CG2 VAL A 100 18.853 2.053 25.591 1.00 6.68 ATOM 700 N ALA A 101 16.277 2.928 1.00 13.14 22.511 15 ATOM 701 CA ALA A 101 16.127 2.266 1.00 15.67 21.183 ATOM ALA A 101 702 C 17.065 2.747 20.053 1.00 12.08 ATOM 703 0 ALA A 101 17.261 4.042 19.907 1.00 11.16 ATOM 704 CB **ALA A 101** 14.685 2.609 20.812 1.00 6.57 MOTA 705 N **GLY A 102** 17.218 1.787 19.099 1.00 7.53 20 атом 706 CA **GLY A 102** 17.949 2.415 17.939 1.00 7.10 MOTA 707 C **GLY A 102** 17.477 1.803 16.744 1.00 7.27 MOTA 708 0 **GLY A 102** 17.102 0.621 16.878 1.00 10.83 ATOM 709 N **GLY A 103** 17.706 2.407 15.648 1.00 7.80 **ATOM** 710 CA **GLY A 103** 17.446 1.745 14.356 1.00 5.33 25 атом 711 C **GLY A 103** 18.303 2.211 13.180 1.00 7.56 ATOM 712 0 **GLY A 103** 18.785 3.340 13.227 1.00 6.88 ATOM 713 N **TYR A 104** 18.490 1.387 12.139 1.00 7.09 MOTA 714 CA **TYR A 104** 19.392 1.682 11.069 1.00 5.99 ATOM 715 С TYR A 104 18.705 1.614 9.705 1.00 9.47 30 ATOM 716 0 TYR A 104 18.115 0.638 9.441 1.00 6.46 **ATOM** 717 CB **TYR A 104** 20.592 0.797 11.079 1.00 5.40 **ATOM** 718 CG TYR A 104 21.436 1.078 9.876 1.00 8.05 ATOM 719 CD1 TYR A 104 21.708 2.302 9.352 1.00 5.91 ATOM 720 CD2 TYR A 104 21.961 -0.044 9.172 6.85 1.00 35 атом 721 CE1 TYR A 104 22.447 2.513 8.186 1.00 5.61 **ATOM** 722 CE2 TYR A 104 22.751 0.052 8.072 1.00 7.49 ATOM 723 CZ**TYR A 104** 22.972 1.377 7.608 1.00 11.08 **ATOM** 724 OH **TYR A 104** 23.795 1.509 6.479 1.00 14.32 **ATOM** 725 N **SER A 105** 18.939 2.975 8.852 1.00 18.39 40 ATOM 726 CA **SER A 105** 18.190 2.854 7.601 1.00 9.66 **ATOM** 727 С **SER A 105** 16.763 2.370 7.722 1.00 6.10 **ATOM** 728 0 **SER A 105** 16.090 3.304 8.077 1.00 5.63 **ATOM** 729 CB **SER A 105** 19.124 2.159 6.607 1.00 8.55 **ATOM** 730 OG **SER A 105** 18.553 1.685 5.463 1.00 24.30 **45** ATOM 731 N **GLN A 106** 16.241 7.079 1.405 1.00 9.93 ATOM 732 CA **GLN A 106** 14.759 1.316 7.002 1.00 8.25 ATOM 733 С **GLN A 106** 14.453 1.089 8.473 1.00 8.51 ATOM 734 0 **GLN A 106** 13.470 1.683 8.862 1.00 6.31 MOTA 735 СВ **GLN A 106** 14.239 0.393 5.940 1.00 7.45 50 ATOM 736 CG **GLN A 106** 13.184 -0.528 6.465 1.00 18.04 MOTA 737 CD **GLN A 106** 12.228 -1.220 5.581 1.00 16.87 **ATOM** 738 OE1 **GLN A 106** 11.024 -1.180 5.492 1.00 17.59 ATOM 739 NE2 GLN A 106 12.643 -2.032 4.713 1.00

ATOM 740 **GLY A 107** N 15.269 0.310 9.172 1.00 7.13 **ATOM** 741 CA **GLY A 107** 15.190 0.159 10.606 1.00 4.61 MOTA 742 C **GLY A 107** 15.048 1.472 11.356 1.00 8.27 **ATOM** 743 0 **GLY A 107** 14.219 1.511 12.290 1.00 6.52 5 атом 744 N ALA A 108 15.653 2.637 11.033 1.00 6.44 ATOM 745 CA **ALA A 108** 15.266 3.864 11.641 1.00 7.41 ATOM С 746 ALA A 108 13.813 4.346 11.471 1.00 11.76 ATOM 747 0 **ALA A 108** 13.150 4.914 12.298 1.00 12.64 ATOM 748 CB **ALA A 108** 16.121 5.006 11.170 1.00 13.93 10 ATOM 749 N ALA A 109 13.321 4.312 10.267 1.00 MOTA 750 CA ALA A 109 12.056 4.685 9.861 1.00 10.47 ATOM 751 C ALA A 109 11.093 3.858 10.727 1.00 12.32 MOTA 752 0 **ALA A 109** 10.016 4.391 11.035 1.00 14.67 ATOM 753 CB ALA A 109 12.035 4.173 8.456 1.00 10.24 **15** ATOM 754 N LEU A 110 11.259 2.690 11.077 1.00 4.34 **ATOM** 755 CA **LEU A 110** 10.458 1.00 11.71 1.760 11.783 MOTA 756 C LEU A 110 10.305 2.253 13.203 1.00 15.26 ATOM 757 0 LEU A 110 9.298 2.672 13.685 1.00 18.07 MOTA 758 CB LEU A 110 11.031 0.319 11.634 1.00 7.52 20 ATOM 759 CG **LEU A 110** 10.247 -0.801 12.258 1.00 8.41 ATOM 760 CD1 LEU A 110 10.685 -2.233 11.862 1.00 7.17 ATOM 761 CD2 LEU A 110 10.278 -0.659 13.783 1.00 5.25 ATOM 762 N ILE A 111 11.397 13.907 2.373 1.00 15.77 ATOM 763 CA ILE A 111 11.510 2.860 15.246 1.00 12.22 25 атом 764 С ILE A 111 11.027 4.255 15.234 1.00 9.39 ATOM 765 0 ILE A 111 10.404 4.636 16.241 1.00 12.54 ATOM ILE A 111 766 CB 12.977 15.685 2.814 1.00 15.55 CG1 ILE A 111 **ATOM** 767 13.222 1.279 15.805 1.00 14.19 ATOM 768 CG2 ILE A 111 13.195 3.465 17:005 1.00 30 атом 769 CD1 ILE A 111 12.410 0.887 17.002 1.00 14.88 ATOM 770 N ALA A 112 11.309 5.170 14.341 1.00 11.00 MOTA 771 CA ALA A 112 10.792 6.528 1.00 12.45 14.427 ATOM 772 ALA A 112 C 9.266 6.455 14.308 1.00 15.59 MOTA 773 0 ALA A 112 8.728 7.131 15.154 1.00 18.13 35 атом 774 CB ALA A 112 11.334 7.505 13.486 1.00 5.70 MOTA 775 N ALA A 113 8.575 5.572 13.587 1.00 12.85 **ATOM** 776 CA **ALA A 113** 7.167 5.512 13.557 1.00 15.39 MOTA 777 С **ALA A 113** 6.475 5.093 14.861 1.00 18.21 ATOM 778 0 **ALA A 113** 5.750 5.498 15.226 1.00 14.59 40 ATOM 779 CB **ALA A 113** 6.678 4.562 12.500 1.00 17.63 MOTA 780 N **ALA A 114** 6.937 3.948 15.303 1.00 16.02 MOTA 781 CA **ALA A 114** 6.483 1.00 16.43 3.218 16.412 ATOM 782 C **ALA A 114** 6.578 4.114 17.643 1.00 22.20 MOTA 783 0 **ALA A 114** 5.673 4.321 18.426 1.00 18.94 45 ATOM 784 CB **ALA A 114** 7.474 2.084 16.565 1.00 4.69 ATOM 785 N VAL A 115 7.722 4.836 17.744 1.00 22.46 **ATOM** 786 CA VAL A 115 7.855 19.064 5.499 1.00 20.88 MOTA 787 С VAL A 115 6.670 6.469 19.007 1.00 22.71 MOTA 788 0 VAL A 115 6.136 6.761 20.057 1.00 22.05 50 атом 789 CB **VAL A 115** 9.279 6.090 19.137 1.00 19.61 **ATOM** 790 CG1 VAL A 115 9.396 7.259 20.122 1.00 8.35 **MOTA** 791 CG2 VAL A 115 10.245 5.016 19.562 1.00 13.91 MOTA 792 N **SER A 116** 6.467 7.085 17.828 1.00 23.59

ATOM 793 CA SER A 116 5.539 8.172 17.736 1.00 23.68 MOTA 794 С **SER A 116** 4.169 7.647 18.120 1.00 23.77 **ATOM** 795 0 **SER A 116** 3.333 8.523 18.399 1.00 27.35 **ATOM** 796 CB **SER A 116** 5.522 8.865 16.376 1.00 25.21 **5** атом 797 OG **SER A 116** 5.168 8.043 15.277 1.00 28.05 **MOTA** 798 N **GLU A 117** 3.859 6.397 18.004 1.00 18.83 ATOM 799 CA **GLU A 117** 2.491 6.020 18.238 1.00 22.21 **ATOM** 800 GLU - A 117 C 2.461 5.474 19.653 1.00 30.46 ATOM 801 0 **GLU A 117** 1.487 4.773 19.863 1.00 35.72 **10** ATOM 802 CB **GLU A 117** 1.977 4.902 17.343 1.00 21.63 ATOM 803 CG **GLU A 117** 2.167 5.219 15.897 1.00 26.41 ATOM 804 CD **GLU A 117** 1.560 4.424 14.814 1.00 34.01 ATOM 805 OE1 GLU A 117 0.912 3.440 15.046 1.00 32.59 ATOM 806 OE2 GLU A 117 1.750 4.833 13.659 1.00 44.62 **15** ATOM 807 N LEU A 118 5.570 3.438 20.512 1.00 34.45 ATOM LEU A 118 808 CA 3.326 5.006 21.812 1.00 33.64 MOTA 809 C LEU A 118 2.681 6.110 22.633 1.00 41.75 ATOM 810 0 **LEU A 118** 2.594 7.267 1.00 39.90 22.370 MOTA 811 CB LEU A 118 4.600 4.668 22.392 1.00 29.44 20 атом 812 CG **LEU A 118** 5.628 3.891 21.645 1.00 26.36 ATOM CD1 LEU A 118 813 6.921 3.840 22.379 1.00 27.53 ATOM CD2 LEU A 118 814 5.110 2.520 21.536 1.00 20.69 MOTA 815 N **SER A 119** 2.076 5.794 23.726 1.00 48.86 ATOM 816 CA **SER A 119** 0.910 5.647 24.476 1.00 52.44 25 атом 817 C **SER A 119** 6.063 25.866 1.212 1.00 52.57 **ATOM** 818 0 **SER A 119** 1.485. 5.258 26.735 1.00 55.54 MOTA 819 CB **SER A 119** 0.550 4.132 24.488 1.00 70.55 ATOM 820 OG SER A 119 1.393 3.091 23.908 1.00 66.80 **ATOM** 821 N **GLY A 120** 1.532 7.307 26.024 1.00 52.95 30 ATOM 822 CA **GLY A 120** 1.910 7.761 27.382 1.00 53.35 **ATOM** 823 С **GLY A 120** 2.944 7.109 28.291 1.00 49.09 MOTA 824 0 **GLY A 120** 4.086 7.617 28.358 1.00 49.66 **ATOM** 825 N ALA A 121 2.526 6.129 29,102 1.00 42.97 826 ATOM CA ALA A 121 3.477 5.574 30.022 1.00 40.72 35 атом 827 C ALA A 121 4.587 4.772 29,326 1.00 44.20 **ATOM** 828 0 ALA A 121 5.749 4.803 29.711 1.00 45.42 MOTA 829 CB ALA A 121 2.965 4.542 30.903 1.00 36.34 **ATOM** 830 N VAL A 122 4.122 4.035 28.312 1.00 41.15 ATOM 831 CA VAL A 122 5.090 3.269 27.548 1.00 33.41 40 ATOM 832 С VAL A 122 5.870 4.168 26.652 1.00 28.48 MOTA 833 0 VAL A 122 7.084 4.019 26.872 1.00 27.69 MOTA 834 CB VAL A 122 4.424 2.056 26.952 1.00 30.22 MOTA 835 CG1 VAL A 122 2.924 1.997 27.098 1.00 28.03 MOTA CG2 VAL A 122 836 4.891 1.836 25.551 1.00 23.22 **45** ATOM 837 N LYS A 123 5.424 5.310 26.177 1.00 23.16 MOTA 838 CA LYS A 123 25.661 6.354 6.314 1.00 23.11 ATOM 839 C LYS A 123 7.403 6.783 26.661 1.00 25.28 MOTA 840 0 LYS A 123 8.524 7.224 26.449 1.00 29.01 **MOTA** 841 CB LYS A 123 5.561 7.502 25.100 1.00 23.54 50 атом 842 CG LYS A 123 6.171 8.573 24.277 1.00 26.71 **ATOM** 843 CD LYS A 123 5.400 9.775 23.888 1.00 43.07 ATOM 844 CE LYS A 123 4.953 9.783 22.461 1.00 59.59 **ATOM** 845 NZ LYS A 123 3.518 9.637 22.099 1.00 67.50

MOTA 846 N **GLU A 124** 6.977 6.991 27.918 1.00 27.95 ATOM 847 CA **GLU A 124** 7.845 7.700 28.863 1.00 27.29 MOTA 848 C **GLU A 124** 8.910 6.706 29.243 1.00 25.21 ATOM 849 0 **GLU A 124** 9.993 7.165 29.769 1.00 21.21 5 ATOM 850 CB **GLU A 124** 6.986 8.351 29.927 1.00 40.13 MOTA 851 CG **GLU A 124** 7.588 8.609 31.295 1.00 57.40 ATOM 852 CD **GLU A 124** 8.530 9.814 31.247 1.00 66.99 MOTA 853 OE1 GLU A 124 9.619 9.751 31.902 1.00 70.44 MOTA 854 OE2 GLU A 124 7.949 10.652 30.502 1.00 73.84 10 ATOM 855 N **GLN A 125** 8.656 5.393 29.058 1.00 19.93 MOTA 856 CA **GLN A 125** 9.761 4.509 29.546 1.00 17.98 MOTA 857 С **GLN A 125** 10.865 4.556 28.521 1.00 24.28 ATOM 858 0 **GLN A 125** 11.964 4.107 28.815 1.00 21.47 **ATOM** 859 CB **GLN A 125** 9.225 3.178 29.844 1.00 9.13 **15** ATOM GLN A 125 9.901 2.001 860 CG 30.299 1.00 9.05 **GLN A 125 ATOM** 861 CD 9.211 0.719 30.129 1.00 19.33 MOTA 862 OE1 GLN A 125 8.190 0.703 29.466 1.00 28.52 MOTA 863 NE2 GLN A 125 -0.396 9.662 30.684 1.00 13.34 VAL A 126 27.319 **ATOM** 864 N 5.188 10.593 1.00 25.30 **20** ATOM 865 CA VAL A 126 26.361 11.738 5.124 1.00 22.55 MOTA C VAL A 126 866 12.546 6.334 26.614 1.00 17.55 MOTA 867 0 VAL A 126 7.408 26.329 12.109 1.00 12.79 ATOM 1.00 23.76 868 CB VAL A 126 11.227 4.560 25.022 MOTA 869 CG1 VAL A 126 9.706 4.686 1.00 23.77 24.946 25 атом 870 CG2 VAL A 126 11.795 5.081 23.743 1.00 23.81 ATOM LYS A 127 871 N 13.726 6.233 27.264 1.00 16.41 MOTA 872 CA LYS A 127 14.462 7.494 27.639 1.00 18.18 ATOM 873 С LYS A 127 15.239 8.063 26.488 1.00 18.49 **ATOM** 874 0 LYS A 127 15.812 9.103 26.680 1.00 18.99 MOTA 06 875 CB LYS A 127 15.401 7.148 28.792 1.00 20.81 **ATOM** 876 CG LYS A 127 14.770 6.110 29.713 1.00 21.99 **ATOM** 877 LYS A 127 CD 13.435 6.726 30.064 1.00 33.86 MOTA 878 CE LYS A 127 12.779 6.612 31.399 1.00 32.17 **ATOM** 879 NZ LYS A 127 12.279 7.863 31.993 1.00 45.34 35 атом 880 1.00 20.56 N **GLY A 128** 15.522 7.281 25.416 MOTA 881 CA **GLY A 128** 16.280 7.948 1.00 20.72 24.306 **ATOM** 882 C **GLY A 128** 16.358 7.104 23.063 1.00 17.71 MOTA 883 0 **GLY A 128** 5.901 16.168 23.226 1.00 16.66 MOTA 884 N VAL A 129 16.451 7.725 21.892 1.00 16.16 40 атом 885 CA VAL A 129 16.497 6.872 20.691 1.00 13.82 VAL A 129 MOTA 886 C 17.519 7.371 19.719 1.00 8.35 MOTA 887 0 VAL A 129 17.602 8.553 19.556 1.00 3.85 MOTA 888 CB VAL A 129 15.192 6.426 20.054 1.00 11.02 MOTA 889 CG1 VAL A 129 14.007 7.041 20.726 1.00 6.50 45 ATOM 890 CG2 VAL A 129 15.051 6.729 18.571 1.00 10.03 MOTA 891 N **ALA A 130** 18.455 6.398 19.363 1.00 8.05 **ATOM** 892 CA **ALA A 130** 19.430 6.845 18.344 1.00 7.55 MOTA 893 С **ALA A 130** 19.078 6.293 16.958 1.00 11.17 MOTA 894 0 **ALA A 130** 18.755 5.145 16.849 1.00 15.74 50 ATOM 895 **ALA A 130** 20.781 CB 6.391 18.603 1.00 5.89 **ATOM** 896 N **LEU A 131** 18.911 6.953 15.892 1.00 7.36 **ATOM** 897 CA LEU A 131 18.635 6.625 14.553 1.00 7.70 MOTA 898 C **LEU A 131** 19.876 6.908 13.661 1.00 12.02

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MOTA 899 0 LEU A 131 20.436 8.033 13.604 1.00 6.80 900 **ATOM** CB LEU A 131 17.604 7.713 14.102 1.00 8.40 MOTA 901 CG LEU A 131 16.160 7.830 14.575 1.00 ATOM 902 CD1 LEU A 131 15.391 8.957 13.981 1.00 5 ATOM 903 CD2 LEU A 131 15.481 6.488 14.324 1.00 5.12 **ATOM** 904 N PHE A 132 20.271 6.009 12.802 1.00 11.56 **ATOM** 905 CA PHE A 132 21.422 6.183 11.908 1.00 10.44 MOTA 906 C PHE A 132 20.965 6.013 10.478 1.00 MOTA 907 0 PHE A 132 20.175 5.101 10.097 1.00 11.04 10 атом 908 4.931 CB PHE A 132 22.217 12.282 1.00 10.56 **ATOM** 909 CG PHE A 132 22.693 4.830 13.714 1.00 16.38 **ATOM** 910 CD1 PHE A 132 21.951 4.029 14.542 1.00 13.36 **ATOM** 911 CD2 PHE A 132 23.860 5.489 14.213 1.00 15.12 **ATOM** 912 CE1 PHE A 132 22.342 3.911 15.889 1.00 14.91 **15** ATOM 913 CE2 PHE A 132 24.176 5.323 15.513 1.00 18.02 MOTA 914 CZPHE A 132 23.426 4.530 16.403 1.00 15.09 **ATOM** 915 N **GLY A 133** 21.431 6.876 9.580 1.00 7.35 **ATOM** 916 CA **GLY A 133** 21.026 6.893 8.148 1.00 5.86 MOTA 917 C **GLY A 133** 19.503 6.919 8.061 1.00 12.25 20 атом **GLY A 133** 918 0 18.890 5.926 7.593 1.00 9.03 MOTA 919 N TYR A 134 18.926 8.070 8.532 1.00 9.85 MOTA 920 CA TYR A 134 17.455 8.022 8.838 1.00 7.40 MOTA 921 С **TYR A 134** 16.647 8.365 7.584 1.00 10.61 MOTA 922 0 TYR A 134 16.785 9.513 7.131 1.00 5.85 25 ATOM 923 CB **TYR A 134** 17.161 9.128 9.836 1.00 7.27 ATOM 924 CG **TYR A 134** 15.842 9.393 10.391 1.00 7.89 MOTA 925 CD1 TYR A 134 14.889 8.437 10.312 1.00 6.65 ATOM 926 CD2 TYR A 134 15.661 10.651 10.948 1.00 11.44 MOTA 927 **CE1 TYR A 134** 13.657 8.690 10.821 1.00 9.05 30 атом 928 CE2 TYR A 134 14.408 10.928 11.467 1.00 12.89 MOTA 929 CZ**TYR A 134** 13.428 9.923 11.423 1.00 14.22 **ATOM** 930 OH **TYR A 134** 12.146 10.110 11.975 1.00 12.41 THR A 135 **ATOM** 931 N 15.811 7.398 7.139 1.00 11.51 MOTA 932 CA THR A 135 15.229 7.581 5.789 1.00 35 атом 933 С THR A 135 14.082 8.530 5.825 1.00 10.36 **ATOM** 934 0 THR A 135 13.845 8.878 4.727 1.00 11.26 ATOM 935 CB THR A 135 14.772 6.394 4.967 1.00 12.02 OG1 THR A 135 MOTA 936 13.821 5.399 5.398 1.00 22.81 **ATOM** 937 CG2 THR A 135 15.828 5.332 4.712 1.00 14.88 40 атом 938 N **GLN A 136** 13.632 9.105 6.928 1.00 15.28 **ATOM** 939 CA **GLN A 136** 12.596 10.134 6.968 1.00 16.48 MOTA 940 C **GLN A 136** 13.102 7.646 11.418 1.00 17.46 GLN A 136 MOTA 941 0 12.292 8.035 12.231 1.00 12.82 ATOM 942 CB **GLN A 136** 11.336 9.671 7.701 1.00 5.71 45 ATOM 943 CG **GLN A 136** 11.178 8.191 7.263 1.00 13.60 MOTA 944 CD **GLN A 136** 10.504 8.264 5.932 1.00 14.65 MOTA 945 OE1 GLN A 136 9.587 9.102 5.986 1.00 23.99 MOTA NE2 GLN A 136 946 10.852 7.529 4.914 1.00 14.68 ATOM 947 N **ASN A 137** 14.421 11.532 7.566 1.00 18.52 50 атом 948 CA **ASN A 137** 14.953 12.752 8.141 1.00 18.16 MOTA C 949 **ASN A 137** 14.301 13.929 7.458 1.00 19.79 **ATOM** 950 o **ASN A 137** 13.895 14.802 8.157 1.00 12.28 MOTA 951 CB **ASN A 137** 16.481 12.573 8.239 1.00 14.17

MOTA 952 CG ASN A 137 17.247 13.740 8.812 1.00 19.75 ATOM 953 OD1 ASN A 137 17.821 14.341 7.934 1.00 14.52 ATOM 954 ND2 ASN A 137 17.390 10.042 14.130 1.00 17.43 ATOM 955 N **LEU A 138** 14.180 14.062 6.141 1.00 27.31 5 атом 956 CA LEU A 138 13.640 15.270 5.553 1.00 25.53 ATOM 957 С **LEU A 138** 12.190 15.332 5.971 1.00 22.45 MOTA 958 0 **LEU A 138** 11.710 6.549 16.281 1.00 25.13 MOTA 959 CB **LEU A 138** 13.632 4.056 1.00 41.28 15.269 ATOM 960 CG **LEU A 138** 13.713 16.582 3.303 1.00 31.76 **10** ATOM 961 CD1 LEU A 138 14.641 4.012 17.503 1.00 51.09 MOTA 962 CD2 LEU A 138 14.207 16.573 1.958 1.00 46.20 ATOM 963 N **GLN A 139** 11.378 14.403 5.569 1.00 20.48 **ATOM** 964 CA **GLN A 139** 10.034 14.390 6.037 1.00 19.98 ATOM 965 C **GLN A 139** 9.846 14.749 7.471 1.00 22.85 **15** ATOM 966 0 **GLN A 139** 8.791 15.282 7.528 1.00 26.66 MOTA 967 CB **GLN A 139** 9.517 12.969 5.899 1.00 18.37 MOTA 968 CG **GLN A 139** 9.684 12.643 4.450 1.00 22.02 MOTA 969 CD **GLN A 139** 10.984 11.983 4.110 1.00 22.69 ATOM 970 OE1 GLN A 139 10.674 10.980 3.477 1.00 35.62 **20** ATOM 971 NE2 GLN A 139 12.195 12.405 4.410 1.00 31.70 MOTA 972 N **ASN A 140** 10.454 14.072 8.427 1.00 26.14 MOTA 973 **ASN A 140** 9.848 CA 10.215 14.183 1.00 19.06 MOTA 974 С **ASN A 140** 10.941 15.429 10.293 1.00 16.99 MOTA 975 11.454 **ASN A 140** 11.040 15.654 1.00 18.05 0 25 атом 976 CB **ASN A 140** 10.581 12.910 10.541 1.00 17.20 **ATOM** 977 CG **ASN A 140** 9.465 11.998 10.210 1.00 16.28 **ATOM** 978 8.615 12.565 9.563 1.00 23.57 OD1 ASN A 140 MOTA 979 ND2 ASN A 140 9.460 10.756 10.630 1.00 22.65 MOTA 980 ARG A 141 9.397 N 11.457 16.162 1.00 19.20 30 атом ARG A 141 9.790 981 CA 12.170 17.350 1.00 26.25 **ATOM** 13.219 982 C ARG A 141 17.090 10.818 1.00 25.06 MOTA 983 0 ARG A 141 13.365 17.928 11.649 1.00 27.60 ATOM 984 CB 11.123 18.299 10.271 1.00 37.72 ARG A 141 **ATOM** 985 CG ARG A 141 10.083 18.974 9.372 1.00 49.61 35 атом 986 1.00 19.42 N **GLY A 142** 14.110 16.165 10.920 MOTA 987 CA **GLY A 142** 14.997 15.778 11.902 1.00 14.21 **ATOM** 988 С **GLY A 142** 14.652 15.066 13.158 1.00 19.42 **ATOM** 989 0 **GLY A 142** 15.547 14.759 13.971 1.00 23.74 MOTA 990 N **GLY A 143** 13.354 14.851 13.569 1.00 14.09 40 ATOM 991 CA **GLY A 143** 14.075 14.757 13.210 1.00 11.80 MOTA C **GLY A 143** 12.972 14.555 992 12.203 1.00 16.69 MOTA 12.787 993 0 **GLY A 143** 11.760 13.481 1.00 19.57 MOTA 994 N ILE A 144 11.668 12.386 15.590 1.00 19.71 **ATOM** 995 CA ILE A 144 10.494 11.589 15.667 1.00 20.13 9.313 **45 ATOM** 996 С **ILE A 144** 12.315 16.296 1.00 27.00 ATOM 13.026 1.00 26.75 997 0 **ILE A 144** 9.298 17.268 ATOM 10.973 10.583 16.692 1.00 16.84 998 CB **ILE A 144** MOTA 12.363 9.956 16.348 1.00 5.60 999 CG1 ILE A 144 **ATOM** 9.882 9.636 16.775 1.00 14.01 1000 CG2 ILE A 144 **50** ATOM 9.156 1.00 2.75 1001 CD1 ILE A 144 12.437 17.562 ATOM 1002 N PRO A 145 8.249 12.380 15.499 1.00 32.77 MOTA 1.00 29.89 1003 CA PRO A 145 6.959 12.993 15.779 ATOM 6.484 12.588 1.00 27.78 1004 C PRO A 145 17.180

MOTA 1005 PRO A 145 6.475 11.446 17.537 0 1.00 26.07 PRO A 145 12.384 14.784 1006 CB 5.957 1.00 26.51 **ATOM** 12.059 MOTA 1007 CG PRO A 145 6.887 13.668 1.00 25.85 **ATOM** 1008 CD PRO A 145 8.174 11.563 14.234 1.00 31.33 **5 ATOM ASN A 146** 5.796 13.462 17.878 1.00 27.07 1009 N MOTA 1010 CA **ASN A 146** 5.454 13.274 19.230 1.00 28.59 **ATOM** 1011 C **ASN A 146** 6.526 12.605 20.045 1.00 29.25 11.995 1.00 35.51 **ATOM** 1012 0 **ASN A 146** 6.087 20.996 ATOM CB 4.285 12.364 19.230 1.00 41.13 1013 **ASN A 146 10** ATOM 3.300 12.568 1014 CG **ASN A 146** 18.120 1.00 48.43 MOTA 1015 OD1 ASN A 146 3.134 13.721 17.788 1.00 49.24 MOTA 1016 ND2 ASN A 146 2.763 11.437 17.695 1.00 47.79 7.791 MOTA 1017 TYR A 147 12.799 19.885 1.00 23.88 N ATOM 8.689 20.969 1.00 21.90 1018 CA **TYR A 147** 12.339 **15** ATOM 1019 TYR A 147 9.583 13.495 21.285 1.00 22.57 C 9.777 MOTA 1020 0 TYR A 147 14.399 20.494 1.00 26.53 20.498 ATOM 1021 CB **TYR A 147** 9.309 11.098 1.00 21.16 MOTA **TYR A 147** 10.285 10.471 21.349 1.00 20.45 1022 CG MOTA 1023 CD1 TYR A 147 9.882 9.720 22.384 1.00 24.28 20 атом 11.608 10.564 21.189 1.00 17.96 1024 CD2 TYR A 147 **ATOM CE1 TYR A 147** 10.681 9.029 23.273 1.00 24.55 1025 12.509 9.948 21.983 1.00 20.73 MOTA 1026 CE2 TYR A 147 23.030 1.00 24.61 **ATOM** 1027 CZ**TYR A 147** 12.022 9.184 ATOM 1028 OH **TYR A 147** 12.891 8.536 23.887 1.00 24.80 **25** атом 9.893 22.507 1.00 22.86 1029 N PRO A 148 13.858 ATOM 1030 PRO A 148 10.817 14.916 22.769 1.00 21.77 CA ATOM 1031 PRO A 148 12.127 14.882 21.957 1.00 22.49 С ATOM 1032 PRO A 148 13.007 14.004 22.117 1.00 22.31 0 ATOM 1033 CB PRO A 148 11.185 14.694 24.251 1.00 23.23 30 ATOM 1034 CG PRO A 148 10.324 13.576 24.719 1.00 23.39 9.677 23.590 1.00 25.33 MOTA 1035 CD PRO A 148 12.889 MOTA N ARG A 149 12.432 15.980 21.250 1.00 25.45 1036 **ATOM** 13.735 16.138 20.567 1.00 22.54 1037 CA ARG A 149 MOTA 21.499 1038 С ARG A 149 14.910 16.018 1.00 21.28 35 ATOM 1039 0 ARG A 149 15.860 15.477 21.015 1.00 16.61 MOTA 13.829 17.346 19.727 1.00 31.02 1040 CB ARG A 149 ATOM 1041 CG ARG A 149 12.837 17.750 18.719 1.00 58.26 13.452 17.658 1.00 80.58 MOTA 1042 CD ARG A 149 18.605 17.798 1.00 92.05 **ATOM** 1043 NE ARG A 149 13.769 16.491 40 ATOM 1.00 91.85 1044 CZARG A 149 13.315 18.154 15.320 19.213 15.165 1.00 86.98 **ATOM** 1045 NH1 ARG A 149 12.586 **ATOM** NH2 ARG A 149 13.544 17.488 14.242 1.00 91.61 1046 ATOM 22.825 1.00 28.09 1047 **GLU A 150** 14.813 16.282 N 23.735 1.00 25.55 **ATOM** 1048 CA **GLU A 150** 15.950 16.171 **45** ATOM 14.736 24.020 1.00 21.12 1049 C **GLU A 150** 16.272 1050 17.372 14.443 24.371 1.00 24.39 **ATOM** 0 **GLU A 150** 24.917 1.00 38.73 17.040 **ATOM** 1051 CB **GLU A 150** 15.753 1.00 67.27 17.370 25.359 **ATOM** 1052 CG **GLU A 150** 14.328 ATOM 1053 CD **GLU A 150** 14.252 17.185 26.899 1.00 85.05 50 атом 1.00 90.70 1054 OE1 GLU A 150 15.005 17.890 27.657 1.00 91.68 **ATOM** OE2 **GLU A 150** 13.454 16.321 27.373 1055 23.727 1.00 19.70 ATOM 1056 N ARG A 151 15.396 13.807 15.752 12.424 23.844 1.00 19.52 MOTA 1057 CA ARG A 151

ATOM 1058 C ARG A 151 16.163 11.779 22.531 1.00 19.28 1059 ARG A 151 16.373 10.586 ATOM 0 22.480 1.00 14.55 **ATOM** 1060 CB ARG A 151 14.548 11.796 24.412 1.00 23.06 ATOM 1061 CG ARG A 151 13.853 12.432 25.516 1.00 22.24 5 атом ARG A 151 1062 CD 13.200 11.451 26.393 1.00 33.40 ARG A 151 12.609 11.893 1.00 46.53 ATOM 1063 NE 27.633 ATOM 1064 ARG A 151 11.796 11.028 28.275 1.00 52.87 CZMOTA 1065 NH1 ARG A 151 11.428 9.823 27.930 1.00 51.02 ARG A 151 MOTA 11.203 11.278 1.00 59.98 1066 NH2 29.416 **10** ATOM 1067 N THR A 152 16.360 12.526 21.505 1.00 14.12 ATOM 1068 THR A 152 16.629 11.925 20.253 1.00 15.05 CA MOTA 1069 C THR A 152 17.995 12.249 19.745 1.00 17.30 1070 18.282 13.373 19.965 **ATOM** 0 THR A 152 1.00 21.34 15.680 MOTA 1071 CB THR A 152 12.408 19.158 1.00 13.91 **15** ATOM 14.423 12.256 19.858 1072 OG1 THR A 152 1.00 23.92 MOTA 1073 CG2 THR A 152 15.737 11.934 17.759 1.00 6.77 19.121 18.704 MOTA 1074 N LYS A 153 11.336 1.00 15.49 MOTA 1075 CA LYS A 153 19.930 11.725 18.450 1.00 17.73 MOTA 1076 C LYS A 153 19.893 11.035 17.073 1.00 18.41 20 ATOM 1077 0 LYS A 153 19.866 9.800 17.121 1.00 16.04 19.338 ATOM 1078 CB LYS A 153 21.112 11.260 1.00 14.55 ATOM 1079 22.523 11.508 18.933 1.00 11.95 CG LYS A 153 ATOM 1080 CD LYS A 153 22.883 12.882 19.403 1.00 40.35 ATOM 1081 CE LYS A 153 24.358 13.093 19.079 1.00 62.12 **25** ATOM 1082 LYS A 153 24.930 14.235 19.863 1.00 73.03 NZ MOTA 1083 VAL A 154 19.910 11.962 16.136 1.00 15.86 N MOTA 1084 CA VAL A 154 20.031 11.508 14.730 1.00 15.79 MOTA 1085 C **VAL A 154** 21.406 11.481 14.040 1.00 13.11 21.958 1.00 13.51 **ATOM** 1086 0 VAL A 154 12.460 13.675 30 ATOM VAL A 154 19.095 12.257 13.674 1.00 5.90 1087 CB ATOM 1088 19.276 11.765 12.247 1.00 8.45 CG1 VAL A 154 ATOM 17.672 12.091 14.117 1.00 7.14 1089 CG2 VAL A 154 ATOM 1090 PHE A 155 22.039 10.448 13.605 1.00 13.75 N 10.473 12.843 1.00 10.67 ATOM 1091 CA PHE A 155 23.263 **35** ATOM 22.906 10.406 11.402 1.00 11.64 1092 C PHE A 155 MOTA 22.505 9.367 10.893 1.00 15.09 1093 0 PHE A 155 23.955 **ATOM** 1094 CB PHE A 155 9.120 13.304 1.00 5.38 **ATOM** 1095 CG PHE A 155 24.396 9.266 14.739 1.00 16.52 ATOM 23.678 8.642 15.696 1.00 23.70 1096 CD1 PHE A 155 40 ATOM 25.503 9.950 15.107 1.00 11.27 1097 CD2 PHE A 155 17.011 24.037 8.702 1.00 23.25 MOTA 1098 CE1 PHE A 155 9.994 MOTA 1099 CE2 PHE A 155 25.888 16.372 1.00 7.37 9.384 1.00 16.13 ATOM 1100 CZ PHE A 155 25.139 17.357 11.255 10.511 1.00 12.38 ATOM CYS A 156 23.205 1101 N **45** ATOM 11.443 9.114 1.00 11.64 1102 CA CYS A 156 22.847 MOTA 1103 CYS A 156 24.057 12.027 8.461 1.00 10.08 C 8.378 1.00 13.73 **ATOM** 1104 0 CYS A 156 24.385 13.174 21.575 12.391 8.917 1.00 6.30 **ATOM** 1105 CYS A 156 CB 8.287 1.00 10.60 ATOM 20.137 11.470 1106 SG CYS A 156 **50** ATOM 24.814 11.147 7.918 1.00 16.95 1107 N **ASN A 157 ATOM** 26.229 11.665 7.576 1.00 19.16 1108 CA **ASN A 157** 12.367 6.310 1.00 17.70 **ATOM** 1109 C **ASN A 157** 26.197 ATOM 1110 0 ASN A 157 25.368 12.330 5.469 1.00 20.91

ATOM 1111 CB **ASN A 157** 27.115 10.714 8.300 1.00 30.34 MOTA 1112 CG **ASN A 157** 27.733 9.498 7.932 1.00 34.95 **ATOM** 1113 OD1 ASN A 157 28.011 8.573 8.606 1.00 44.28 ATOM 1114 ND2 ASN A 157 27.965 9.541 6.660 1.00 54.18 5 атом 1115 N VAL A 158 26.849 13.501 6.313 1.00 25.65 ATOM 1116 CA VAL A 158 26.825 14.483 5.192 1.00 28.21 MOTA 1117 C VAL A 158 26.768 13.893 3.758 1.00 24.85 MOTA 1118 0 VAL A 158 25.732 14.266 3.111 1.00 30.96 MOTA 1119 CB VAL A 158 27.954 15.512 5.217 1.00 27.87 **10 ATOM** CG1 VAL A 158 1120 28.751 14.595 4.238 1.00 40.51 MOTA 1121 CG2 VAL A 158 27.791 16.704 4.399 1.00 34.39 MOTA 1122 N **GLY A 159** 27.483 12.956 3.016 1.00 5.94 MOTA 1123 CA **GLY A 159** 26.713 12.774 1.732 1.00 6.20 ATOM 1124 C **GLY A 159** 25.734 11.797 1.487 1.00 4.00 **15** ATOM 1125 0 **GLY A 159** 25.732 10.704 0.848 1.00 4.06 ATOM 1126 N **ASP A 160** 25.052 11.441 2.643 1.00 8.53 **ATOM** 1127 CA **ASP A 160** 24.106 10.302 2.828 1.00 11.97 **ATOM** 1128 C **ASP A 160** 22.755 10.698 2.177 1.00 14.44 ATOM 1129 0 **ASP A 160** 21.928 11.398 2.692 1.00 10.21 20 атом 1130 CB ASP A 160 24.037 9.829 4.277 1.00 12.43 MOTA 1131 CG **ASP A 160** 23.126 8.629 4.261 1.00 20.99 **ATOM** 1132 OD1 ASP A 160 22.525 8.408 3.179 1.00 33.03 MOTA OD2 ASP A 160 1133 22.956 7.840 5.216 1.00 10.13 MOTA 1134 N ALA A 161 22.455 10.402 0.961 1.00 12.33 25 атом 1135 CA ALA A 161 21.318 10.743 0.269 1.00 11.01 MOTA 1136 C ALA A 161 19.961 10.317 0.848 1.00 15.22 ATOM 1137 0 ALA A 161 18.969 11.034 0.594 1.00 9.50 MOTA 1138 CB ALA A 161 21.365 10.334 -1.172 1.00 13.68 ATOM 1139 N VAL A 162 19.915 9.468 1.840 1.00 14.54 30 атом 1140 CA VAL A 162 18.653 9.014 2.287 1.00 9.86 MOTA 1141 C VAL A 162 18.235 10.063 3.258 1.00 13.50 MOTA VAL A 162 1142 0 17.094 10.458 3.377 1.00 20.47 MOTA VAL A 162 1143 CB 18.596 7.778 3.117 1.00 7.34 MOTA 1144 CG1 VAL A 162 18.931 6.592 2.259 1.00 6.50 35 атом 1145 CG2 VAL A 162 19.514 7.858 4.210 1.00 18.46 MOTA 1146 N CYS A 163 19.198 10.733 3.719 1.00 13.44 **ATOM** 1147 CA CYS A 163 18.864 11.811 4.720 1.00 11.26 MOTA 1148 C CYS A 163 18.256 12.963 4.042 1.00 15.57 MOTA 1149 0 CYS A 163 18.219 13.857 4.880 1.00 14.09 40 атом 1150 CB CYS A 163 12.145 20.144 5.570 1.00 18.70 **MOTA** 1151 SG CYS A 163 20.748 10.705 6.581 1.00 13.38 ATOM 1152 N THR A 164 18.100 13.014 2.696 1.00 21.82 ATOM 1153 CA THR A 164 17.603 14.283 2.171 1.00 23.08 MOTA 1154 С THR A 164 16.597 14.022 1.098 1.00 23.39 **45** атом 1155 0 THR A 164 16.517 14.727 0.137 1.00 33.37 ATOM 1156 CB THR A 164 18.463 15.341 1.454 1.00 23.25 MOTA 1157 OG1 THR A 164 19.486 14.707 0.674 1.00 23.21 ATOM 1158 CG2 THR A 164 18.958 16.261 2.491 1.00 37.71 ATOM 1159 N **GLY A 165** 15.802 13.085 1.309 1.00 24.23 **50** ATOM 1160 CA **GLY A 165** 14.606 12.783 0.579 1.00 26.69 **ATOM** 1161 C **GLY A 165** 14.699 11.814 -0.515 1.00 28.56 **ATOM** 1162 0 **GLY A 165** 13.680 11.775 -1.124 1.00 39.76 **ATOM** 1163 N THR A 166 15.661 11.044 -0.736 1.00 25.80

ATOM 1164 CA THR A 166 16.006 10.220 -1.774 1.00 25.53 **ATOM** 1165 С THR A 166 16.195 8.866 -1.175 1.00 25.35 ATOM 1166 0 THR A 166 16.913 8.760 -0.206 1.00 30.91 ATOM 1167 CB THR A 166 17.406 10.657 -2.230 1.00 31.57 5 атом 1168 OG1 THR A 166 17.105 11.788 -2.982 1.00 24.13 ATOM 1169 CG2 THR A 166 18.061 9.559 -2.983 1.00 34.67 **ATOM** 1170 N **LEU A 167** 15.734 7.833 -1.817 1.00 19.63 **ATOM** 1171 CA **LEU A 167** 6.552 16.219 -1.465 1.00 16.11 MOTA 1172 С **LEU A 167** 17.395 6.044 -2.300 1.00 19.87 10 атом 1173 0 **LEU A 167** 17.265 4.869 -2.612 1.00 21.38 **ATOM** 1174 CB **LEU A 167** 15.086 5.624 -1.555 1.00 23.45 MOTA 1175 ÇG **LEU A 167** 14.123 5.773 -0.401 1.00 33.91 MOTA 1176 CD1 LEU A 167 12.969 4.908 -0.793 1.00 42.10 ATOM 1177 CD2 LEU A 167 14.776 5.385 0.903 1.00 25.86 **15** ATOM 1178 N ILE A 168 18.534 6.726 -2.507 1.00 21.67 ATOM 1179 ILE A 168 CA 19.608 6.051 -3.170 1.00 23.38 MOTA 1180 ILE A 168 C 20.675 5.585 -2.189 1.00 20.47 MOTA 1181 0 ILE A 168 21.139 6.541 -1.581 1.00 18.08 **ATOM** 1182 CB ILE A 168 20.254 6.835 -4.297 1.00 23.50 20 атом 1183 CG1 ILE A 168 21.232 7.874 -3.800 1.00 13.71 ATOM CG2 ILE A 168 1184 19.445 7.627 -5.276 1.00 18.16 ATOM 1185 CD1 ILE A 168 20.908 8:938 -4.804 1.00 26.95 ATOM 1186 N ILE A 169 21.396 4.478 -2.394 1.00 18.32 MOTA 1187 CA ILE A 169 22.554 4.448 -1.536 1.00 13.25 25 атом 1188 С ILE A 169 23.924 4.662 -1.967 1.00 11.95 **ATOM** 1189 0 ILE A 169 24.615 3.942 -2.539 1.00 20.35 ATOM 1190 CB ILE A 169 22.503 3.351 -0.499 1.00 21.07 MOTA 1191 CG1 ILE A 169 23.398 2.181 -0.655 1.00 11.06 MOTA 1192 CG2 ILE A 169 21.122 2.801 -0.533 1.00 7.02 30 атом 1193 CD1 ILE A 169 22.581 1.266 -1.587 1.00 32.83 MOTA 1194 N THR A 170 24.570 5.586 -1.296 1.00 17.16 MOTA 1195 THR A 170 CA 25.883 6.217 -1.3971.00 13.01 ATOM 1196 C THR A 170 26.722 5.719 -0.240 1.00 10.14 MOTA 1197 0 THR A 170 26.334 5.036 0.758 1.00 9.98 35 атом 1198 CB THR A 170 25.623 -1.344 7.713 1.00 15.02 MOTA 1199 OG1 THR A 170 26.466 7.947 -0.255 1.00 23.39 CG2 THR A 170 MOTA 1200 24.389 7.914 -0.452 1.00 41.10 MOTA 1201 PRO A 171 N 28.000 5.738 -0.469 1.00 10.12 ATOM 1202 CA PRO A 171 29.012 5.066 0.339 1.00 11.88 40 ATOM 1203 С PRO A 171 28.897 5.492 1.765 1.00 9.74 **ATOM** 1204 0 PRO A 171 28.904 4.682 2.646 1.00 9.54 MOTA PRO A 171 1205 CB 30.414 5.207 -0.286 1.00 7.15 **ATOM** 1206 CG PRO A 171 30.017 5.603 -1.654 1.00 7.18 ATOM 1207 CD PRO A 171 28.667 6.233 -1.601 1.00 6.90 **45** атом 1208 N ALA A 172 28.725 6.718 1.980 1.00 6.71 MOTA 1209 CA ALA A 172 28.247 7.315 3.169 1.00 MOTA 1210 С ALA A 172 27.075 6.631 3.892 1.00 10.99 **ATOM** 1211 0 ALA A 172 27.037 6.755 5.165 1.00 16.49 MOTA 1212 CB ALA A 172 27.904 8.812 3.040 1.00 2.86 50 атом HIS A 173 1213 N 26.287 5.815 3.278 1.00 6.36 **ATOM** 1214 CA HIS A 173 25.133 5.468 4.081 1.00 5.29 ATOM 1215 С HIS A 173 25.685 4.314 4.888 1.00 10.58 ATOM 1216 0 HIS A 173 25.082 3.598 5.668 1.00 9.36

ATOM 1217 CB HIS A 173 24.081 4.883 3.216 1.00 ATOM 1218 CG HIS A 173 22.815 4.403 3.791 1.00 7.30 **ATOM** 1219 ND1 HIS A 173 22.066 5.327 4.565 1.00 8.48 **ATOM** 1220 CD2 HIS A 173 22.148 3.264 3.670 1.00 7.83 5 ATOM 1221 CE1 HIS A 173 20.932 4.657 4.861 1.00 17.36 ATOM 1222 NE2 HIS A 173 20.945 3.423 4.379 1.00 5.29 ATOM 1223 N **LEU A 174** 26.823 3.947 4.326 1.00 8.03 MOTA 1224 CA **LEU A 174** 27.344 2.623 4.682 1.00 ATOM 1225 C **LEU A 174** 28.171 2.787 5.930 1.00 13.06 **10** ATOM 1226 0 **LEU A 174** 28.609 1.648 6.151 1.00 19.88 MOTA LEU A 174 1227 CB 28.078 2.118 3.488 1.00 2.76 ATOM 1228 CG **LEU A 174** 27.560 0.902 2.847 1.00 13.35 MOTA 1229 CD1 LEU A 174 26.024 1.017 2.796 1.00 18.01 **ATOM** 1.00 21.70 1230 CD2 LEU A 174 27.913 0.740 1.421 **15 ATOM** 1231 N **SER A 175** 28.290 3.989 6.447 1.00 12.43 ATOM CA 1232 **SER A 175** 29.230 4.052 7.553 1.00 18.01 MOTA C 1233 **SER A 175** 28.872 4.811 8.847 1.00 19.89 MOTA 1234 0 **SER A 175** 28.968 6.047 9.120 1.00 14.61 ATOM 1235 CB **SER A 175** 4.606 30.516 6.847 1.00 20.11 20 ATOM 1236 OG **SER A 175** 30.834 5.907 7.293 1.00 27.73 MOTA 1237 N **TYR A 176** 28.479 3.978 9.815 1.00 17.89 1238 CA MOTA **TYR A 176** 28.092 4.530 11.133 1.00 12.54 **ATOM** 1239 C **TYR A 176** 28.530 3.671 12.272 1.00 11.16 MOTA 1240 0 **TYR A 176** 27.949 3.770 13.257 1.00 7.63 25 атом 1241 CB **TYR A 176** 26.511 1.00 9.13 4.283 11.053 **ATOM** 1242 CG TYR A 176 25.831 5.525 10.029 1.00 5.03 **ATOM** 1243 CD1 TYR A 176 25.874 6.923 10.425 1.00 2.75 ATOM 1244 CD2 TYR A 176 5.022 8.980 25.152 1.00 2.18 MOTA 1245 **CE1 TYR A 176** 25.287 7.754 9.633 1.00 4.25 30 ATOM 1246 CE2 TYR A 176 24.649 5.981 8.085 1.00 6.77 **ATOM** 1247 CZ **TYR A 176** 24.658 7.329 8.399 1.00 6.22 ATOM 1248 OH **TYR A 176** 24.074 8.375 7.635 1.00 5.76 **ATOM** 1249 N THR A 177 29.430 2.685 12.167 1.00 10.72 MOTA 1250 CA THR A 177 29.797 1.854 13.284 1.00 13.31 35 атом 1251 C THR A 177 30.516 2.659 14.320 1.00 12.46 MOTA 1252 0 THR A 177 30.311 2.436 15.475 1.00 13.12 ATOM 1253 CB THR A 177 30.658 0.683 12.798 1.00 3.49 MOTA 1254 OG1 THR A 177 31.361 1.247 11.870 1.00 32.08 ATOM 1255 CG2 THR A 177 29.675 -0.149 12.083 1.00 6.42 40 ATOM 1256 N **ILE A 178** 31.409 3.474 13.920 1.00 10.48 ATOM 1257 CA **ILE A 178** 32.203 4.246 14.783 1.00 15.25 MOTA 1258 C ILE A 178 5.045 15.632 31.180 1.00 16.95 MOTA 1259 0 **ILE A 178** 31.092 4.774 16.851 1.00 22.68 **ATOM** 1260 CB ILE A 178 33.338 5.121 14.357 1.00 25.11 45 ATOM 1261 CG1 ILE A 178 34.701 4.496 14.056 1.00 25.05 MOTA CG2 ILE A 178 1262 33.599 6.205 15.392 1.00 27.60 **ATOM** 1263 CD1 ILE A 178 34.553 3.006 14.071 1.00 55.86 **ATOM** 1264 N **GLU A 179** 30.218 5.799 15.178 1.00 16.34 ATOM 1265 CA **GLU A 179** 6.610 15.985 29.290 1.00 16.94 **50** ATOM 1266 С GLU A 179 28.324 5.713 16.692 1.00 14.79 **ATOM** 1267 0 **GLU A 179** 27.683 6.012 17.716 1.00 19.20 MOTA 1268 CB **GLU A 179** 28.555 7.637 15.169 1.00 21.16 ATOM 1269 CG **GLU A 179** 28.790 7.283 13.691 1.00 50.37

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                 cz
                     ARG A 186
                                      32.324
                                               8.346
                                                       22.870
                                                                1.00 50.20
   MOTA
           1321
                 NH1 ARG A 186
                                      31.924
                                               9.538
                                                       22.424
                                                                1.00 47.65
   MOTA
           1322
                 NH2 ARG A 186
                                      33.115
                                               7.476
                                                      22.318
                                                               1.00 39.90
```

**ATOM** 1323 N PHE A 187 25.565 8.774 24.434 1.00 8.37 MOTA 1324 PHE A 187 CA 24.195 9.370 24.426 1.00 13.48 MOTA 1325 PHE A 187 C 23.187 8.476 25.182 1.00 15.92 ATOM 1326 0 PHE A 187 22.379 8.916 25.995 1.00 14.81 5 атом 1327 CB PHE A 187 23.667 9.791 23.087 1.00 11.81 MOTA 1328 CG PHE A 187 22.282 10.323 23.032 1.00 14.64 ATOM 1329 CD1 PHE A 187 21.984 11.586 23.391 1.00 8.47 ATOM CD2 PHE A 187 1330 21.186 9.599 22.564 1.00 18.34 **ATOM** 12.134 23.353 1331 CE1 PHE A 187 20.698 1.00 12.89 10 ATOM 22.485 1332 CE2 PHE A 187 19.895 10.026 1.00 17.42 **ATOM** 1333 CZ11.322 PHE A 187 19.661 22.924 1.00 3.70 ATOM 1334 N **LEU A 188** 23.033 7.232 24.803 1.00 15.17 ATOM 1335 CA **LEU A 188** 21.908 6.427 25.324 1.00 18.43 ATOM 1336 C LEU A 188 22.207 6.221 26.775 1.00 19.67 **15** ATOM 1337 O **LEU A 188** 21.280 6.512 27.461 1.00 18.17 MOTA 1338 CB **LEU A 188** 21.703 5.088 24.552 1.00 18.72 ATOM 1339 CG **LEU A 188** 21.116 5.375 23.136 1.00 9.96 MOTA 1340 CD1 LEU A 188 20.950 4.066 22.601 1.00 7.86 **ATOM** 1341 CD2 LEU A 188 19.849 6.206 23.168 1.00 4.70 20 атом ARG A 189 1342 N 23.333 5.805 27.230 1.00 17.48 **ATOM** 1343 CA ARG A 189 23.798 5.812 28.547 1.00 18.41 **ATOM** 1344 C ARG A 189 23.353 7.039 29.321 1.00 16.87 MOTA 1345 0 ARG A 189 22.852 7.164 30.389 1.00 13.64 ATOM 1346 СВ ARG A 189 25.325 6.017 28.529 1.00 21.93 25 атом 1347 CG ARG A 189 25.882 5.624 29.894 1.00 19.95 MOTA 1348 CD ARG A 189 27.239 6.140 30.235 1.00 21.42 MOTA 1349 NE ARG A 189 27.257 7.545 29.926 1.00 25.62 ATOM 1350 CZARG A 189 28.491 7.983 29.699 1.00 29.22 MOTA 1351 NH1 ARG A 189 29.315 6.960 29.840 1.00 26.71 30 атом 1352 NH2 ARG A 189 28.780 9.210 29.383 1.00 33.27 MOTA 1353 N ASP A 190 23.837 8.150 28.796 1.00 13.76 **ATOM** 1354 CA **ASP A 190** 23.489 9.338 29.615 1.00 17.78 **ATOM** 1355 C **ASP A 190** 22.008 29.711 9.364 1.00 16.79 ATOM 1356 0 **ASP A 190** 21.661 9.891 30.692 1.00 23.13 35 ATOM 1357 CB **ASP A 190** 23.995 10.663 29.070 1.00 23.17 ATOM 1358 CG **ASP A 190** 25.553 10.664 29.079 1.00 33.40 **ATOM** 1359 OD1 ASP A 190 26.250 9.836 29.761 1.00 22.68 ATOM 1360 OD2 ASP A 190 25.961 11.595 28.321 1.00 30.24 ATOM 1361 N ARG A 191 21.156 9.128 28.781 1.00 21.61 40 ATOM 1362 CA ARG A 191 19.707 9.265 28.849 1.00 20.99 ATOM 1363 C ARG A 191 19.176 8.237 29.825 1.00 21.23 ATOM 1364 ARG A 191 0 18.327 8.515 30.651 1.00 20.98 ATOM 1365 CB ARG A 191 19.014 9.214 27.450 1.00 19.76 **ATOM** 1366 CG ARG A 191 19.605 10.282 26.521 1.00 27.49 **45** ATOM 1367 CD ARG A 191 18.848 11.594 26.689 1.00 36.68 ATOM ARG A 191 1368 NE 17.559 11.023 27.144 1.00 60.89 ATOM 1369 czARG A 191 11.651 28.087 1.00 73.30 16.841 MOTA 1370 NH1 ARG A 191 17.404 12.780 28.496 1.00 76.65 ATOM 1371 NH2 ARG A 191 28.574 15.675 11.224 1.00 62.02 50 атом 7.037 1372 N **ILE A 192** 19.734 29.885 1.00 21.02 ATOM 1373 CA ILE A 192 19.500 6.080 30.913 1.00 21.92 MOTA 1374 C **ILE A 192** 19.705 6.598 32.337 1.00 25.67 MOTA 1375 0 ILE A 192 19.145 6.053 33.263 1.00 27.95

5677-000, SLK, 1998-12-04

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|    | MOTA | 1376 | CB  | ILE A | 192 | 20.289 | 4.775  | 30.750 | 1.00 24.23 |
|----|------|------|-----|-------|-----|--------|--------|--------|------------|
|    | MOTA | 1377 | CG1 | ILE A | 192 | 19.770 | 4.215  | 29.475 | 1.00 26.91 |
|    | ATOM | 1378 | CG2 | ILE A | 192 | 19.923 | 3.983  | 31.951 | 1.00 15.15 |
|    | ATOM | 1379 | CD1 | ILE A | 192 | 20.418 | 2.954  | 29.019 | 1.00 21.07 |
| 5  | ATOM | 1380 | N   | ARG A | 193 | 20.535 | 7.574  | 32.629 | 1.00 28.72 |
|    | ATOM | 1381 | CA  | ARG A | 193 | 20.800 | 8.068  | 33.963 | 1.00 33.95 |
|    | ATOM | 1382 | C   | ARG A | 193 | 20.116 | 9.377  | 34.406 | 1.00 42.87 |
|    | MOTA | 1383 | 0   | ARG A | 193 | 20.479 | 9.267  | 35.618 | 1.00 48.19 |
|    | ATOM | 1384 | CB  | ARG A | 193 | 22.298 | 8.179  | 34.167 | 1.00 34.19 |
| 10 | ATOM | 1385 | CG  | ARG A | 193 | 23.096 | 6.896  | 34.100 | 1.00 39.38 |
|    | ATOM | 1386 | CD  | ARG A | 193 | 24.590 | 7.213  | 34.133 | 1.00 65.92 |
|    | ATOM | 1387 | NE  | ARG A | 193 | 25.339 | 5.973  | 34.003 | 1.00 81.05 |
|    | ATOM | 1388 | CZ  | ARG A | 193 | 26.631 | 5,765  | 33.770 | 1.00 81.52 |
| 15 | MOTA | 1389 | NH1 | ARG A | 193 | 27.441 | 6.816  | 33.647 | 1.00 80.92 |
|    | MOTA | 1390 | NH2 | ARG A | 193 | 27.120 | 4.536  | 33.652 | 1.00 74.00 |
|    | ATOM | 1391 | OT  | ARG A | 193 | 19.292 | 10.277 | 34.082 | 1.00 38.80 |
|    | TER  |      |     |       |     |        |        |        |            |